

Temperature Dependence of Physical-Chemical Properties of Selected Chemicals of Environmental Interest. II. Chlorobenzenes, Polychlorinated Biphenyls, Polychlorinated Dibenzo-*p*-dioxins, and Dibenzofurans

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Data are compiled and reviewed of the physical-chemical properties of chlorinated benzenes, biphenyls, and dibenzo-*p*-dioxins and dibenzofurans, which control air-water partitioning, namely vapor pressure, aqueous solubility, and Henry's law constant over the environmentally relevant temperature range of 5–50 °C. Recommended values at 25 °C, and equations for estimating these properties over the temperature range of 5–50 °C are provided. Corresponding enthalpies of phase transition are also reported.
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Key words: air-water partition coefficient, aqueous solubility, chlorinated dibenzofurans, chlorinated dibenzo-*p*-dioxins, chlorobenzenes, Henry's law constant, PCBs, physical-chemical properties, temperature dependence, vapor pressure.

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1. Introduction

This is Part II of a two part review of the environmentally relevant properties of aromatic compounds with emphasis on the temperature dependence of vapor pressure, aqueous solubility and Henry's law constant. Part I [Shiu and Ma (2000)] which addresses mononuclear and polynuclear aromatic hydrocarbons includes a discussion of the incentive for such a review and provides an account of the thermodynamic relationships between these quantities. Expressions for temperature dependence are reviewed and the approach described by which experimental data were acquired and subjected to critical review with the intent of selecting recommended values, and in some cases recommended equations. The reader is referred to Part I for full details.

Briefly, experimental data were gathered for each compound including enthalpies of fusion, vaporization and sublimation, and the data were tabulated giving the method of measurement. The focus was on the temperature range of 5–50 °C. These data were plotted as logarithm of the property (such as aqueous solubility) versus reciprocal absolute temperature, and following a critical review, a property value, with 95% confidence limits, was selected at 25 °C. Where possible, equations were suggested expressing temperature dependence. The selected values and equations were consolidated in separate tables. In some cases reported equations are recommended, in others the data were regressed to obtain a new equation, and for some compounds it was judged that the data were insufficient in quality and quantity to permit an equation to be recommended. For the substances addressed here the aqueous solubility is so low that it is considered valid to assume that the Henry's law constant is equal to the ratio of vapor pressure and aqueous solubility. Equations are given, where possible, for vapor pressure and solubility from which the reader can derive the equation for Henry's law constant. No equation is thus presented for this property.

The reader is cautioned to exercise care when using reported data to ensure that the phase (solid or liquid) of the substances is specified. Most of the substances treated here are solids. Many of the reported data apply to the liquid state, having been obtained by extrapolation from higher temperatures, or representing measurement of the supercooled state, for example by GC retention time. Care should be taken to ensure which state applies and avoid erroneously estimating the Henry's law constant as the ratio of, for example, a supercooled liquid vapor pressure to a solid solubility. For many of the substances addressed here the only available data apply to the supercooled state, and it is the property in this state for which quantitative structure property relationships (QSPRs) are sought and reported.

2. Data Compilation and Presentation

As in the previous paper, only experimentally measured vapor pressures, aqueous solubilities and Henry's law constants are reported. Data which are calculated or estimated

TABLE I. Physical constants and thermodynamic properties of chlorinated aromatic hydrocarbons

TABLE I. Physical constants and thermodynamic properties of chlorinated aromatic hydrocarbons—Continued

Compound	CAS No.	Formula	MW	mp/°C	bp/°C	$\Delta_{\text{fus}}H$ kJ·mol ⁻¹	t/°C	Reference	$\Delta_{\text{vap}}H$ kJ·mol ⁻¹	$\Delta_{\text{sub}}H$ kJ·mol ⁻¹	t/°C	Reference
1,2,4 TCB (cont'd)												
1,3,5-Trichlorobenzene	108-70-3	C ₆ H ₃ Cl ₃	181.45	64	208	15.48		Tsonopoulos & Prausnitz 71	58.06	25		Grovers <i>et al.</i> 1990
								Plato & Glasgow 1969	46.91			Weast 1982–83
								Tsonopoulos 1970	19.62			Grovers <i>et al.</i> 1990
								Tsonopoulos & Prausnitz 71	19.92			Weast 1982–83
1,2,3,4-Tetrachlorobenzene	634-66-2	C ₆ H ₂ Cl ₄	215.9	47.5	254	17		Miller <i>et al.</i> 1984	53.86			Grovers <i>et al.</i> 1990
1,2,3,5-Tetrachlorobenzene	634-90-2	C ₆ H ₂ Cl ₄	215.9	54.5	246	19		Miller <i>et al.</i> 1984	50.13			Weast 1982–83
1,2,4,5-Tetrachlorobenzene	95-94-3	C ₆ H ₂ Cl ₄	215.9	140	243	24.1		Miller <i>et al.</i> 1984	53.68			Grovers <i>et al.</i> 1990
Pentachlorobenzene	608-93-5	C ₆ HCl ₅	250.3	86	277	20.6		Miller <i>et al.</i> 1984	63.59			Weast 1982–83
Hexachlorobenzene	118-74-1	C ₆ Cl ₆	284.8	230	322	16.1		Oppenhuizen <i>et al.</i> 1987	63.28			Grovers <i>et al.</i> 1990
								Plato & Glasgow 1969				Weast 1982–83
								Tsonopoulos 1970				Grovers <i>et al.</i> 1990
								Miller <i>et al.</i> 1984				Weast 1982–83
								Dean 1985	101.25			Grovers <i>et al.</i> 1990
									105			Liu & Dickhut 1994
								Oppenhuizen <i>et al.</i> 1987				Dickhut <i>et al.</i> 1987
PCBs:												
2-chlorobiphenyl	2051-60-7	C ₁₂ H ₉ Cl	188.7	34		14.52		Geidarov <i>et al.</i> 1975	57.78			Geidarov <i>et al.</i> 1975
3-chlorobiphenyl	2051-61-8	C ₁₂ H ₉ Cl	188.7	25.1		15.3		Miller <i>et al.</i> 1984	79.4			Ferro <i>et al.</i> 1983
4-chlorobiphenyl	2051-62-9	C ₁₂ H ₉ Cl	188.7	77.9		13.32		Geidarov <i>et al.</i> 1975	69.2			Ferro <i>et al.</i> 1983
								Dickhut <i>et al.</i> 1987	65.94			Geidarov <i>et al.</i> 1975
								Oppenhuizen <i>et al.</i> 1987	79.24			Burkhard <i>et al.</i> 1984
									70.8			Ferro <i>et al.</i> 1983
									77.4			Wania <i>et al.</i> 1994
									86			Smith <i>et al.</i> 1964
									96.2			Smith <i>et al.</i> 1964
2,2'-dichloro- 2,5-dichloro- 4,4'-dichloro-	34883-39-1	C ₁₂ H ₈ Cl ₂	223.1	61					93.9			Wania <i>et al.</i> 1994
2,2',3,3'-trichloro- 2,4,5-trichloro- 2,4,6-trichloro- 2,2',5,5'-tetrachloro-	2050-68-2	C ₁₂ H ₈ Cl ₂	223.1	25.1					93.9			Geidarov <i>et al.</i> 1975
2,4,4'-trichloro- 2,4,5-trichloro- 2,4,6-trichloro- 2,2',5,5'-tetrachloro-	34883-39-1	C ₁₂ H ₈ Cl ₂	223.1	149					90.8			Dickhut <i>et al.</i> 1987
2,3,4,5-tetrachloro- 3,3',4,4'-tetrachloro-	32598-13-3	C ₁₂ H ₈ Cl ₂	292	87					105			Oppenhuizen <i>et al.</i> 1987
2,2',4,5,5'-pentachloro- 2,2',3,3',6,6'-hexachloro-	37680-73-2	C ₁₂ H ₅ Cl ₅	326.4	76.5					103.7			Miller <i>et al.</i> 1984
2,2',3,3',6,6'-hexachloro-	38411-22-2	C ₁₂ H ₄ Cl ₆	360.9	112.2					95.3			Oppenhuizen <i>et al.</i> 1987
2,2',4,4',5,5'-hexachloro- 2,2',4,4',6,6'-hexachloro-	35065-27-1	C ₁₂ H ₄ Cl ₆	360.9	103					103.7			Miller <i>et al.</i> 1984
2,2',3,3',5,5'-octaCB	33979-03-2	C ₁₂ H ₄ Cl ₆	360.9	114					101.7			Oppenhuizen <i>et al.</i> 1987
	2136-99-4	C ₁₂ H ₂ Cl ₈	429.7	162					101.7			Miller <i>et al.</i> 1984
									22.6			Dickhut <i>et al.</i> 1987

TABLE 1. Physical constants and thermodynamic properties of chlorinated aromatic hydrocarbons—Continued

Compound	CAS No.	Formula	MW	mp/°C	bp/°C	$\Delta_{\text{fus}}H$ kJ·mol ⁻¹	t/°C	Reference	$\Delta_{\text{vap}}H$ kJ·mol ⁻¹	t/°C	$\Delta_{\text{sub}}H$ kJ·mol ⁻¹	t/°C	Reference
2,2',3,3',4,4',5,5',6-nonaCB decachlorobiphenyl	40186-72-9 2051-24-3	C ₁₂ HCl ₉ C ₁₂ Cl ₁₀	464.2 498.7	206 305.9	26.0 26.3 28.70 28.70	Opperhuizen <i>et al.</i> 1987 Opperhuizen <i>et al.</i> 1987 Miller <i>et al.</i> 1984 Dickhut <i>et al.</i> 1987 Opperhuizen <i>et al.</i> 1987	Oppenhuizen <i>et al.</i> 1987 Oppenhuizen <i>et al.</i> 1987 Miller <i>et al.</i> 1984 Dickhut <i>et al.</i> 1987 Oppenhuizen <i>et al.</i> 1987	121.8	Burkhardt <i>et al.</i> 1984				
Dioxins: dibenzo-p-dioxin	262-23-4	C ₁₂ H ₈ O ₂	184	122-123*	283.5	22.6	mp	Rordorf 1986, 1989	68.4	mp	92.25	Rordorf 1986, 1989	
1-chloro-	39227-53-7	C ₁₂ H ₇ O ₂ Cl	218.5	104.5-105.5*	315.5	21.4	mp	Rordorf 1986, 1989	76.2	mp	98.55	Rordorf 1986, 1989	
2-chloro-	39227-54-8	C ₁₂ H ₇ O ₂ Cl	218.5	89-89*	316	18.5	mp	Rordorf 1986, 1989	78.1	mp	97.16	Rordorf 1986, 1989	
2,3-dichloro-	29446-15-9	C ₁₂ H ₆ O ₂ Cl ₂	253	163-164*	358	26.7	mp	Rordorf 1986, 1989	77.8	mp	97.16	Rordorf 1986, 1989	
2,7-dichloro-	33857-26-0	C ₁₂ H ₆ O ₂ Cl ₂	253	209-210*	373.5	26.8	mp	Rordorf 1986, 1989	76.4	mp	105.51	Rordorf 1986, 1989	
2,8-dichloro-	38964-22-6	C ₁₂ H ₆ O ₂ Cl ₂	253	150.5-151*	209#	23.3	mp	Rordorf 1986, 1989	84.1	mp	109.01	Rordorf 1986, 1989	
1,2,4-trichloro-	39227-58-2	C ₁₂ H ₅ O ₂ Cl ₃	287.5	128-129*	275	33.9	mp	Rordorf 1986, 1989	83.9	mp	118.79	Rordorf 1986, 1989	
1,2,3,4-tetrachloro-	30746-58-8	C ₁₂ H ₄ O ₂ Cl ₄	322	189*	419	31.2	mp	Rordorf 1986, 1989	85.6	mp	118.53	Rordorf 1986, 1989	
1,2,3,7-TCDD	67028-18-6	C ₁₂ H ₄ O ₂ Cl ₄	322	175\$	438.3	36.6	mp	Rordorf 1986, 1989	89.42	25	Grovers <i>et al.</i> 1990		
1,3,6,8-tetrachloro-	30746-58-8	C ₁₂ H ₄ O ₂ Cl ₄	322	219-219.5*	438.3	36.6	mp	Friesen & Webster 1990 Chiou & Manes 1990	90.9	mp	129.41	Rordorf 1986, 1989	
2,3,7,8-TCDD	1746-01-6	C ₁₂ H ₄ O ₂ Cl ₄	322	305-306*	446.5	38.91	mp	Schroy <i>et al.</i> 1985a Rordorf 1986, 1989	86.5	mp	125.794	Rordorf 1986, 1989	
1,2,3,4,7-	39227-61-7	C ₁₂ H ₃ O ₂ Cl ₅	356.4	195-196*	464.7	42.4	mp	Rordorf 1986, 1989	85	mp	115-125	Rordorf 1986, 1989	
1,2,3,4,6,7,8-	39227-26-8	C ₁₂ H ₂ O ₂ Cl ₆	391	275*	487.7	48.1	mp	Friesen <i>et al.</i> 1990	71.81	bp	123.91	Schroy <i>et al.</i> 1985a, b	
1,2,3,4,6,7-	35822-46-9	C ₁₂ HO ₂ Cl ₇	425.2	265\$	507.2	26.0	mp	Chiou & Manes 1990	69.9	mp	124.001	Schroy <i>et al.</i> 1985a, b	
octachlorodibenzo-p-dioxin	3268-87-9	C ₁₂ O ₂ Cl ₈	460	330*	510	30.4	mp	Friesen <i>et al.</i> 1990	92.5	mp	137.419	Rordorf 1986, 1989	
Dibenzofurans: dibenzofuran	132-64-9	C ₁₂ H ₈ O	168.2	86.5	287	19.6	mp	Rordorf 1989	106.9	25	149.792	Grovers <i>et al.</i> 1990	
									89.1	mp	137.419	Rordorf 1986, 1989	
									102.4	25	137.419	Grovers <i>et al.</i> 1990	
									96.75	25	124.001	Rordorf 1986, 1989	
									122.8	mp	137.419	Grovers <i>et al.</i> 1990	
									90.1	mp	124.001	Rordorf 1986, 1989	
									106.9	25	137.419	Grovers <i>et al.</i> 1990	
									111.9	25	151.13	Rordorf 1986, 1989	
									65.4	mp	85.63	Grovers <i>et al.</i> 1990	
												Rordorf 1986, 1989	

TABLE 1. Physical constants and thermodynamic properties of chlorinated aromatic hydrocarbons—Continued

Compound	CAS No.	Formula	MW	mp/°C	bp/°C	$\Delta_{\text{fus}}H$ kJ·mol ⁻¹	t/°C	Reference	$\Delta_{\text{vap}}H$ kJ·mol ⁻¹	$t/^\circ\text{C}$	$\Delta_{\text{sub}}H$ kJ·mol ⁻¹	t/°C	Reference
2,8-dichloro-	5409-83-6	C ₁₂ H ₆ OCl ₂	237.1	184	375	25.1	mp	Rordorf 1986, 1989	74.2	mp	101.432	Rordorf 1989	
1,2,3,4-TCDF	24478-72-6	C ₁₂ H ₄ OCl ₄	306	168.5		36.6	mp	Rordorf 1989	84.2	mp	122.826	Rordorf 1989	
2,3,7,8-TCDF	51207-31-9	C ₁₂ H ₄ OCl ₄	306	227	438.3	36.6	mp	Rordorf 1989	80.3	mp	119.699	Rordorf 1989	
octachlorodibenzofuran	39001-02-0	C ₁₂ OCl ₈	433.8	258	537	57.5	mp	Rordorf 1986, 1989	90	mp	149.43	Rordorf 1986, 1989	

Note:

 $\Delta_{\text{fus}}H$ - enthalpy of fusion $\Delta_{\text{vap}}H$ - enthalpy of vaporization $\Delta_{\text{sub}}H$ - enthalpy of sublimation

mp - melting in °C

bp - boiling point in °C

*mp from Pohland and Yang 1972

\$ mp from Friesen *et al.* 1985

mp from Rordorf 1987

TABLE 2. Aqueous solubilities and reported equations of chlorobenzenes, chlorinated dioxins and dibenzofurans

Compound	t/°C	Solubility (g/m ³)	Method	Reference
chlorobenzene	30	488	shake flask-interferometry	Gross & Sayler 1931
	25.5	1100	shake flask	Othmer <i>et al.</i> 1941
	25	4000	shake flask	Newman <i>et al.</i> 1949
	25	500	shake flask-UV	Andrews & Keefer 1950
	30	490	shake flask-vapor phase	Kisarov 1962
	40	705		
	50	960		
	60	1100		
	70	1605		
	80	1805		
	90	2500		
	21	534	shake flask-GC	Chey & Calder 1972
	25	462.4	shake flask-spectrophotometry	Vesala 1974
	5	40	shake flask-GC	Nelson & Smit 1978
	25	106.8		
	35	267.4		
	45	400.5		
	25	471.3	shake flask-GC	Aquan-Yuen <i>et al.</i> 1979
	25	503	shake flask-UV	Yalkowsky <i>et al.</i> 1979
	10	440	elution chromatography	Schwarz & Miller 1980
	20	420		
	30	490		
	10	460	shake flask-UV	
	20	450		
	30	500		
$S/(g/kg) = 11.3351 - 3.029 \times 10^{-2} \cdot T - 1.8716 \times 10^{-2} \cdot T^2 + 0.559466 \times 10^{-7} \cdot T^3$				Horvath & Getzen 1985
correlated polynomial eq. using exptl data from literature, range 283–363 K				
1,2-dichlorobenzene	25	295	gen. col.-HPLC/UV	Tewari <i>et al.</i> 1982
	25	474	shake flask-head space-GC	McNally & Grob 1983
	25	499	gen. col.-HPLC	Wasik <i>et al.</i> 1983
	25	295	gen. col.-GC	Miller <i>et al.</i> 1984
	25	502	shake flask-UV	Banerjee 1984
	25	350	shake flask-radiometry	Lo <i>et al.</i> 1986
	20	482	VLE-activity coeff.	Cooling <i>et al.</i> 1992
	30	608		
	40	840		
	50	1263		
	25	496	SPME-GC/ECD	Paschke <i>et al.</i> 1998
	25	333	shake flask-GC/MS	Boyd <i>et al.</i> 1998
	recommended value at 25 °C: 484 ± 20 g·m ⁻³			
	20	134	volumetric	Klemenc & Löw 1930
	25	145		
	30	161		
	35	183		
	40	194		
	45	203		
	55	223		
	60	232		
	0	133	shake flask-GC/ECD	Chiou & Freed 1977
	20	148		
	34	162		
	10	169	elution chromatography	Schwarz & Miller 1980
	20	128		
	10	156	shake flask-UV	
	20	124		
	25	156	shake flask-LSC	Banerjee <i>et al.</i> 1980
	25	154	shake flask-GC/ECD	Chiou <i>et al.</i> 1982
$S/(g/kg) = 19.2314 - 0.18114 \cdot T + 5.6509 \times 10^{-4} \cdot T^2 - 5.77683 \times 10^{-7} \cdot T^3$				Horvath & Getzen 1985
correlated polynomial eq. using exptl data from literature, 273–333 K				
2,3-dichlorobenzene	25	149.4	shake flask-head space-GC	McNally & Grob 1983
	25	92.3	gen. col.-HPLC	Miller <i>et al.</i> 1984
	25	137	shake flask-HPLC	Banerjee 1984
	25	169	radiometric	Lo <i>et al.</i> 1986
	25	152.9	shake flask-GC/ECD	Tam <i>et al.</i> 1996

TABLE 2. Aqueous solubilities and reported equations of chlorobenzenes, chlorinated dioxins and dibenzofurans—Continued

Compound	<i>t</i> /°C	Solubility (g/m ³)	Method	Reference
1,2-DCB (cont'd)	25	97.0	SPME-GC/ECD	Paschke <i>et al.</i> 1998
	25	109	shake flask-GC/MS	Boyd <i>et al.</i> 1998
	recommended value at 25 °C: 140±10 g·m ⁻³			
1,3-dichlorobenzene	20	111	volumetric	Klemenc & Löw 1930
	25	123		
	30	140		
	35	150		
	40	167		
	45	177		
	55	196		
	60	201		
	25	102.9	shake flask-UV	Vesala 1974
	25	119.5	shake flask-UV	Yalkowsky <i>et al.</i> 1979
	23.5	149	elution chromatography	Schwarz 1980
	23.5	144		
	10	116	elution chromatography	Schwarz & Miller 1980
	20	89		
	30	133		
	10	118	shake flask-UV	
	20	101		
	30	135		
	25	133.5	shake flask-LSC	Banerjee <i>et al.</i> 1980
	25	134.1	shake flask-GC/ECD	Chiou <i>et al.</i> 1982
	25	235.5	shake flask-head space-GC	McNally & Grob 1983
	25	124.5	gen. col.-HPLC	Miller <i>et al.</i> 1984
	25	143	shake flask-UV	Banerjee 1984
	<i>S</i> /(g/kg)=27.6827-0.261 597· <i>T</i> +8.197 06×10 ⁻⁴ · <i>T</i> ² -8.4698×10 ⁻⁷ · <i>T</i> ³			Horvath & Getzen 1985
	correlated polynomial eq. using exptl data from lit., range 283-333 K			
	25	138	shake flask-GC/MS	Boyd <i>et al.</i> 1998
	recommended value at 25 °C: 120±10 g·m ⁻³			
1,4-dichlorobenzene	20	68.9	volumetric	Klemenc & Löw 1930
Δ _{so} H/kJ·mol ⁻¹		79.1		
18.2	5-45 °C	Shiu <i>et al.</i> 1997		
	30	93.3		
	35	104		
	35	83		
	40	101		
	45	122		
	30	77	shake flask	Gross & Sayler 1931
	25	76	shake flask-UV	Andrews & Keefer 1950
	22.2	77.8	shake flask-UV	Wauchope & Getzen 1972
	24.6	83.4		
	25.5	86.9		
	30	92.6		
	34.5	102		
	38.4	121		
	47.5	169		
	50.1	173		
	25	85.5	shake flask-GC	Vesala 1974
	20	56.9	shake flask-GC	Chiou & Freed 1977
	25	87.15	shake flask-GC/FID	Aquan-Yuen <i>et al.</i> 1979
	25	90.6	shake flask-UV	Yalkowsky <i>et al.</i> 1979
	25	73.8	shake flask-LSC	Banerjee <i>et al.</i> 1980
	25	48.1	shake flask-GC	Könemann 1981
	25	73.0	shake flask-GC	Chiou <i>et al.</i> 1982
	25	92.13	shake flask-head space-GC	McNally & Grob 1983
	25	30.9	gen. col.-HPLC	Miller <i>et al.</i> 1984
	25	65.3	shake flask-HPLC	Banerjee 1984
	<i>S</i> /(g/kg)=13.974-0.085 829· <i>T</i> +0.000 133 65· <i>T</i> ²			Horvath & Getzen 1985
	correlated polynomial eq. using exptl data from lit., 328-348 K			
	22	9.70	shake flask-GC/ECD	Nyssen <i>et al.</i> 1987
	25	10.13		
	5	48.6	shake flask-GC/ECD	Shiu <i>et al.</i> 1997
	15	63		

TABLE 2. Aqueous solubilities and reported equations of chlorobenzenes, chlorinated dioxins and dibenzofurans—Continued

Compound	<i>t</i> /°C	Solubility (g/m ³)	Method	Reference
1,4-DCB (cont'd)	25	81.4		
	35	104.5		
	45	130		
	25	42	shake flask-GC/MS	Boyd <i>et al.</i> 1998
	recommended value at 25 °C: 80±5 g·m ⁻³			
1,2,3-trichlorobenzene	25	31.5	shake flask-UV	Yalkowsky <i>et al.</i> 1979
$\Delta_{\text{sol}}H/\text{kJ} \cdot \text{mol}^{-1}$	25	16.6	shake flask-GC/FID	Mackay & Shiu 1981
28.8	5–45 °C	Shiu <i>et al.</i> 1997	25	Könemann 1981
			25	Miller <i>et al.</i> 1984
			23	Chiou 1985
			25	Chiou <i>et al.</i> 1986
			5	Shiu <i>et al.</i> 1997
			25	19.31
			50	45.61
			25	23.7
			25	13
	recommended value at 25 °C: 21±5 g·m ⁻³			
1,2,4-trichlorobenzene	25	34.7	shake flask-UV	Yalkowsky <i>et al.</i> 1979
	25	19.4	shake flask-GC	Könemann 1981
	25	48.8	shake flask-GC	Chiou <i>et al.</i> 1982
	25	64.31	shake flask-GC	McNally & Grob 1983
	25	46.1	gen. col.-GC/ECD	Miller <i>et al.</i> 1984
	25	31.3	shake flask-HPLC	Banerjee 1984
	25	34.6	shake flask-GC	Chiou 1985
	25	44.8	shake flask-GC/ECD	Tam <i>et al.</i> 1996
	25	52.0	shake flask-GC/MS	Boyd <i>et al.</i> 1998
	recommended value at 25 °C: 40±10 g·m ⁻³			
1,3,5-trichlorobenzene	25	6.59	shake flask-UV	Yalkowsky <i>et al.</i> 1979
$\Delta_{\text{sol}}H/\text{kJ} \cdot \text{mol}^{-1}$	25	5.87	shake flask-GC	Könemann 1981
22.04	5–45 °C	Shiu <i>et al.</i> 1997	25	Miller <i>et al.</i> 1984
			25	Banerjee 1984
			25	Chiou 1985
			5	Shiu <i>et al.</i> 1997
			15	6.29
			25	8.46
			35	11.14
			45	15.55
			25	2.40
	recommended value at 25 °C: 8.0±3 g·m ⁻³			Boyd <i>et al.</i> 1998
1,2,3,4-TeCB	25	4.31	shake flask-UV	Yalkowsky <i>et al.</i> 1979
	25	3.42	shake flask-GC	Könemann 1981
	25	12.2	gen. col.-GC/ECD	Miller <i>et al.</i> 1984
	23	7.18	shake flask-GC	Chiou 1985
	25	3.27	shake flask-GC/ECD	Kim & Saleh 1990
	25	2.20	shake flask-GC/MS	Boyd <i>et al.</i> 1998
	recommended value at 25 °C: 7.0±3 g·m ⁻³			
1,2,3,5-TeCB	25	3.50	shake flask-UV	Yalkowsky <i>et al.</i> 1979
$\Delta_{\text{sol}}H/\text{kJ} \cdot \text{mol}^{-1}$	25	4.02	shake flask-LSC	Banerjee <i>et al.</i> 1980
26.3	5–45 °C	Shiu <i>et al.</i> 1997	25	Veith <i>et al.</i> 1980
			25	Könemann 1981
			25	Banerjee 1984
			23	Miller <i>et al.</i> 1984
			25	Chiou 1985
			25	Doucette & Andren 1988
			25	Kim & Saleh 1990
			25	Tam <i>et al.</i> 1996
			5	Shiu <i>et al.</i> 1997
			15	2.43
			25	3.44
			35	5.08
			45	7.03
			25	3.79
	recommended value at 25 °C: 3.5±1.0 g·m ⁻³			Shiu <i>et al.</i> 1997

TABLE 2. Aqueous solubilities and reported equations of chlorobenzenes, chlorinated dioxins and dibenzofurans—Continued

Compound		t/°C	Solubility (g/m ³)	Method	Reference
1,2,4,5-TeCB $\Delta_{\text{sol}}H/\text{kJ}\cdot\text{mol}^{-1}$ 30.8	5–45 °C Shiu <i>et al.</i> 1997	25	0.595	shake flask-UV	Yalkowsky <i>et al.</i> 1979
		25	0.29	shake flask-GC	Könemann 1981
		25	2.35	gen. col.-GC/ECD	Miller <i>et al.</i> 1984
		25	0.465	shake flask-HPLC	Banerjee 1984
		25	0.56	shake flask-GC/ECD	Kim & Saleh 1990
		5	0.208	gen. col.-GC/ECD	Shiu <i>et al.</i> 1997
		15	0.322		
		25	0.528		
		35	0.739		
		45	1.127		
pentachlorobenzene $\Delta_{\text{sol}}H/\text{kJ}\cdot\text{mol}^{-1}$ 31.3	5–45 °C Shiu <i>et al.</i> 1997	25	2.20	shake flask-GC/MS	Boyd <i>et al.</i> 1998
		recommended value at 25 °C: 0.60±0.1 g·m ⁻³			
		25	0.56	shake flask-UV	Yalkowsky <i>et al.</i> 1979
		25	1.33	shake flask-LSC	Banerjee <i>et al.</i> 1980
		25	1.34	shake flask-LSC	Veith <i>et al.</i> 1980
		25	0.24	shake flask-GC	Könemann 1981
		25	0.831	gen. col.-GC/ECD	Miller <i>et al.</i> 1984
		23	0.385	shake flask-GC/ECD	Chiou 1985
		22	0.18	gen. col.-GC/ECD	Opperhuizen <i>et al.</i> 1985
		23	0.19	shake flask-HPLC	Li & Yalkowsky 1994
hexachlorobenzene $\Delta_{\text{sol}}H/\text{kJ}\cdot\text{mol}^{-1}$ 36.9	5–45 °C Shiu <i>et al.</i> 1997	5	0.145	gen. col.-GC/ECD	Shiu <i>et al.</i> 1997
		15	0.254		
		25	0.419		
		35	0.618		
		45	0.856		
		25	0.447	shake flask-GC/ECD	Shiu <i>et al.</i> 1997
		25	0.87	shake flask-GC/MS	Boyd <i>et al.</i> 1998
		recommended value at 25 °C: 0.50±0.2 g·m ⁻³			
		25	0.005	gen. col.-GC/ECD	Weil <i>et al.</i> 1974
		25	0.006	shake flask-LSC	Lu & Metcalf 1975
Polychlorinated biphenyls (PCBs): 2-chlorobiphenyl	Opperhuizen <i>et al.</i> 1987	25	0.11	shake flask-nephelometric	Hollifield 1979
		25	0.005	shake flask-UV	Yalkowsky <i>et al.</i> 1979
		25	0.0039	shake flask-GC	Könemann 1981
		25	0.0054	shake flask-GC/ECD	Hashimoto <i>et al.</i> 1982
		25	0.047	gen. col.-GC/ECD	Miller <i>et al.</i> 1984
		23	0.0052	shake flask-HPLC	Li & Yalkowsky 1994
		5	0.0022	gen. col.-GC/ECD	Shiu <i>et al.</i> 1997
		15	0.0035		
		25	0.00544		
		35	0.00853		
4-chlorobiphenyl $\Delta_{\text{sol}}H/\text{kJ}\cdot\text{mol}^{-1}$ 28.5	4–32 °C Stolzenburg & Andren 83	45	0.014		
		25	0.005	SPME-GC/ECD	Paschke <i>et al.</i> 1998
		25	0.38	shake flask-GC/MS	Boyd <i>et al.</i> 1998
		recommended value at 25 °C: 0.005±0.05 g·m ⁻³			
		25	5.90	shake flask-GC	Wallnöfer <i>et al.</i> 1973
		25	4.13	gen. col.-GC	Weil <i>et al.</i> 1974
		20	5.08	shake flask-GC	Chiou <i>et al.</i> 1983
		25	7.80	shake flask	Neely 1983
		25	5.056	gen. col.-GC	Miller <i>et al.</i> 1984
		recommended value at 25 °C: 5.5±0.5 g·m ⁻³			
28.45	4–32 °C Dickhut <i>et al.</i> 1986	25	1.17	shake flask-GC	Wallnöffer <i>et al.</i> 1973
		25	1.40	shake flask-GC	Hutzinger <i>et al.</i> 1974
		25	0.90	gen. col.-GC/ECD	Weil <i>et al.</i> 1974
		4	0.631	gen. col.-GC/ECD	Stolzenburg & Andren 1983
28.5	4–32 °C Doucette & Andren 1988	20	1.15		
24.5	5–45 °C Shiu <i>et al.</i> 1997	25	1.41		
		32	2.03		
		$S/(\text{mol/L}) = 2.94 \times 10^{-6} \cdot \exp(0.041 \cdot t)$			

TABLE 2. Aqueous solubilities and reported equations of chlorobenzenes, chlorinated dioxins and dibenzofurans—Continued

Compound	<i>t</i> /°C	Solubility (g/m ³)	Method	Reference		
4-CBP (cont'd)	25	1.20	shake flask-GC	Neely 1983		
	25	1.30	gen. col.-HPLC/UV	Billington <i>et al.</i> 1988		
	25	1.38				
	25	1.336	gen. col.-GC/ECD	Li <i>et al.</i> 1992		
	25	1.334	gen. col.-GC/ECD	Li & Doucette 1993		
	5	0.822	gen. col.-GC/ECD	Shiu <i>et al.</i> 1997		
	15	1.07				
	25	1.37				
	35	2.17				
	45	3.04				
	recommended value at 25 °C: 1.5±0.30 g·m ⁻³					
2,2'-dichlorobiphenyl	25	1.50	shake flask	Wallnöfer <i>et al.</i> 1973		
	25	0.790	gen. col.-GC	Weil <i>et al.</i> 1974		
	20	0.82	shake flask-GC/ECD	Chiou <i>et al.</i> 1983		
	25	1.207	gen. col.-GC/ECD	Dunnivant & Elzerman 1988		
	recommended value at 25 °C:					
2,4'-dichlorobiphenyl	25	1.88	shake flask-GC	Wallnöfer <i>et al.</i> 1973		
	25	0.637	gen. col.-GC/ECD	Weil <i>et al.</i> 1974		
	25	0.62	shake flask-GC	Haque & Schmedding 1975		
	25	0.139	shake flask-GC	Lee <i>et al.</i> 1979		
	20	1.17	shake flask-GC/ECD	Chiou <i>et al.</i> 1983		
	recommended value at 25°C:					
4,4'-dichloro-	25	0.080	shake flask	Wallnöfer <i>et al.</i> 1973		
$\Delta_{\text{sol}}H/\text{kJ}\cdot\text{mol}^{-1}$	25	0.056	gen. col.-GC/ECD	Weil <i>et al.</i> 1974		
40.2	5–45 °C	Shiu <i>et al.</i> 1997	20	0.062	shake flask-GC/ECD	Chiou <i>et al.</i> 1977
			25	0.058	gen. col.-GC/ECD	Billington <i>et al.</i> 1988
			25	0.048		Dunnivant & Elzerman 1988
			25	0.0363	gen. col.-GC	Shiu <i>et al.</i> 1997
			5	0.0210	gen. col.-GC/ECD	
			15	0.0346		
			25	0.057		
			35	0.106		
			45	0.186		
	recommended value at 25 °C: 0.055±0.01 g·m ⁻³					
2,2',5-trichloro-	25	0.64	gen.col.-GC	Weil <i>et al.</i> 1974		
	25	0.248	shake flask	Haque & Schmedding 1975		
	25	0.51	gen. col.-GC	Dunnivant & Elzerman 1988		
	recommended value at 25 °C: 0.40±20 g·m ⁻³					
2,4,4'-trichloro-	25	0.085	shake flask-GC	Wallnöfer <i>et al.</i> 1973		
	25	0.260	gen. col.-GC/ECD	Weil <i>et al.</i> 1974		
	20	0.115	shake flask-GC/ECD	Chiou <i>et al.</i> 1983		
	25	0.116	shake flask-GC/ECD	Chiou <i>et al.</i> 1986		
	recommended value at 25 °C:					
2,4,5-trichloro-	25	0.092	gen. col.-GC/ECD	Weil <i>et al.</i> 1974		
$\Delta_{\text{sol}}H/\text{kJ}\cdot\text{mol}^{-1}$	25	0.162	gen. col.-GC/ECD	Miller <i>et al.</i> 1984		
36.9	5–45 °C	Shiu <i>et al.</i> 1997	5	0.0413	gen. col.-GC/ECD	Shiu <i>et al.</i> 1997
			15	0.0682		
			25	0.106		
			35	0.203		
			45	0.33		
	recommended value at 25 °C: 0.140±0.02 g·m ⁻³					
2,4,6-trichloro-	25	0.226	gen. col.-GC/ECD	Miller <i>et al.</i> 1984		
$\Delta_{\text{sol}}H/\text{kJ}\cdot\text{mol}^{-1}$	4	0.0803	gen. col.-GC/ECD	Doucette & Andren 1988		
33.5	4–32 °C	Doucette & Andren 1988	25	0.1867		
			40	0.4326		
	$S/(\text{mol/L}) = 2.49 \times 10^{-7} \cdot \exp(0.047 \cdot t)$					
	25	0.251	gen. col.-GC	Dunnivant & Elzerman 1988		
	25	0.2403	gen. col.-GC/ECD	Li <i>et al.</i> 1992		

TABLE 2. Aqueous solubilities and reported equations of chlorobenzenes, chlorinated dioxins and dibenzofurans—Continued

Compound	t/°C	Solubility (g/m ³)	Method	Reference		
2,4,6-TCB (cont'd)	25	0.2173	gen. col.-GC/ECD	Li & Andren 1994		
	recommended value at 25 °C: 0.20±0.02 g·m ⁻³					
2,2',5,5'-tetrachloro-	25	0.046	shake flask-GC	Wallnöfer <i>et al.</i> 1973		
	25	0.0265	shake flask-GC	Haque & Schmedding 1975		
	25	0.016	shake flask-LSC	Metcalf <i>et al.</i> 1975		
	16.5	0.006 01	shake flask-GC	Wiese & Griffin 1978		
	25	0.0223	shake flask-GC	Lee <i>et al.</i> 1979		
	25	0.055	gen. col.-GC	Bruggman <i>et al.</i> 1981		
	25	0.027	gen. col.-GC/ECD	Miller <i>et al.</i> 1984		
	25	0.17	gen. col.-HPLC	Billington <i>et al.</i> 1988		
	25	0.011	gen. col.-GC/ECD	Dunnivant & Elzerman 1988		
	22	0.011	gen. col.-GC/ECD	Opperhuizen <i>et al.</i> 1988		
	recommended value at 25 °C: 0.030±0.015 g·m ⁻³					
2,3,4,5-tetrachloro-	25	0.0192	gen. col.-GC/ECD	Weil <i>et al.</i> 1974		
Δ _{sol} H/kJ·mol ⁻¹	25	0.0209	shake flask-GC	Haque & Schmedding 1975		
41.3	5–45 °C	Shiu <i>et al.</i> 1997	25	0.0209	gen. col.-GC/ECD	Miller <i>et al.</i> 1984
			25	0.0099	gen. col.-HPLC/UV	Billington <i>et al.</i> 1988
			25	0.014	gen. col.-GC	Dunnivant & Elzerman 1988
			5	0.0056	gen. col.-GC/ECD	Shiu <i>et al.</i> 1997
			15	0.0102		
			25	0.0156		
			35	0.0285		
			45	0.056		
	recommended value at 25 °C: 0.020±0.005 g·m ⁻³					
3,3',4,4'-tetrachloro-	25	0.175	shake flask-GC/ECD	Wallnöfer <i>et al.</i> 1973		
Δ _{sol} H/kJ·mol ⁻¹	25	7.50×10 ⁻⁴	gen. col.-GC/ECD	Weil <i>et al.</i> 1974		
50.7	4–32 °C	Dickhut <i>et al.</i> 1986	4	1.46×10 ⁻⁴	gen. col.-GC/ECD	Dickhut <i>et al.</i> 1986
			20	4.38×10 ⁻⁴		
50.5	4–32 °C	Doucette & Andren 1988	36	5.84×10 ⁻⁴		
			32	1.17×10 ⁻³		
	$S/(mol\cdot L^{-1}) = 3.59 \times 10^{-10} \cdot \exp(0.007 \cdot t)$					
		22	1.80×10 ⁻³	gen. col.-GC/ECD	Opperhuizen <i>et al.</i> 1988	
		25	5.49×10 ⁻⁴	gen. col.-GC/ECD	Dunnivant & Elzerman 1988	
		25	6.10×10 ⁻⁴	gen. col.-GC/ECD	Hong and Qiao 1995	
	recommended value at 25 °C: (8.0±1)×10 ⁻⁴ g·m ⁻³					
2,2',4,5,5'-pentachloro-	25	0.031	shake flask-GC	Wallnöfer <i>et al.</i> 1973		
Δ _{sol} H/kJ·mol ⁻¹	25	0.0042	gen. col.-GC/ECD	Weil <i>et al.</i> 1974		
45.6	4–32 °C	Dickhut <i>et al.</i> 1986	25	0.0103	shake flask-GC	Haque & Schmedding 1975
31.8	4–32 °C	Doucette & Andren 1988	24	0.010	shake flask-GC	Chiou <i>et al.</i> 1977
			16.5	0.00424	shake flask-GC	Wiese & Griffin 1978
			25	0.0189	gen. col.-GC/ECD	Miller <i>et al.</i> 1984
			25	0.0110	shake flask-GC/ECD	Chiou <i>et al.</i> 1986
			20	0.0026		Murphy <i>et al.</i> 1987
			4	0.0061	gen. col.-GC/ECD	Dickhut <i>et al.</i> 1986
			20	0.0121		
			25	0.0154		
			32	0.0223		
	$S/(mol\cdot L^{-1}) = 1.54 \times 10^{-8} \cdot \exp(0.046 \cdot t)$					
		25	0.006 76	gen. col.-GC/ECD	Dunnivant & Elzerman 1988	
	recommended value at 25 °C: 0.015±0.005 g·m ⁻³					

TABLE 2. Aqueous solubilities and reported equations of chlorobenzenes, chlorinated dioxins and dibenzofurans—Continued

Compound			<i>t</i> /°C	Solubility (g/m ³)	Method	Reference
2,2',4,4',5,5'-hexa- $\Delta_{\text{sol}}H/\text{kJ}\cdot\text{mol}^{-1}$ 20.3	4–32 °C	Doucette & Andren 1988	25	8.80×10^{-3}	shake flask-GC	Wallnöfer <i>et al.</i> 1973
			25	1.20×10^{-4}	gen. col.-GC/ECD	Weil <i>et al.</i> 1974
			25	0.000 953	shake flask-GC	Haque & Schmedding 1975
			24	0.000 95	shake flask-GC	Chiou <i>et al.</i> 1977
			16.5	1.05×10^{-4}	shake flask-GC	Wiese & Griffin 1978
			4	4.62×10^{-3}	gen. col.-GC/ECD	Doucette & Andren 1988
			25	8.45×10^{-3}		
			40	1.28×10^{-2}		
			$S/(\text{mol/L}) = 1.15 \times 10^{-8} \cdot \exp(0.028 \cdot t)$			
			22	1.15×10^{-3}	gen. col.-GC/ECD	Opperhuizen <i>et al.</i> 1988
2,2',3,3',6,6'-hexa- $\Delta_{\text{sol}}H/\text{kJ}\cdot\text{mol}^{-1}$ 50.7	4–25 °C	Dickhut <i>et al.</i> 1986	25	0.006 03	gen. col.-GC/ECD	Miller <i>et al.</i> 1984
			20	0.0020		Murphy <i>et al.</i> 1987
			4	1.2×10^{-3}	gen.col.-GC/ECD	Dickhut <i>et al.</i> , 1986
			20	3.25×10^{-3}		
			25	4.51×10^{-3}		
			$S/(\text{mol/L}) = 2.39 \times 10^{-9} \cdot \exp(0.065 \cdot t)$			
			recommended value at 25 °C: $(0.85 \pm 0.05) \times 10^{-3} \text{ g}\cdot\text{m}^{-3}$			
			25	0.0099	shake flask-GC	Dexter & Pavlou 1978
			25	0.000 20		
45.5	4–25 °C	Doucette & Andren 1988	22	2.80×10^{-3}	gen. col.-LSC	Coyle <i>et al.</i> 1997
			recommended value at 25 °C: $(0.85 \pm 0.05) \times 10^{-3} \text{ g}\cdot\text{m}^{-3}$			
			25	0.000 99	shake flask-GC	
			25	0.000 03	gen. col.-GC/ECD	
			20	0.0020		
			4	1.2×10^{-3}	gen.col.-GC/ECD	
			20	3.25×10^{-3}		
			25	4.51×10^{-3}		
			$S/(\text{mol/L}) = 2.39 \times 10^{-9} \cdot \exp(0.065 \cdot t)$			
34.2	5–45 °C	Shiu <i>et al.</i> 1997	recommended value at 25 °C: $0.004 \pm 0.002 \text{ g}\cdot\text{m}^{-3}$			
			25	9.00×10^{-4}	gen. col.-GC/ECD	Weil <i>et al.</i> 1974
			25	4.10×10^{-4}	gen. col.-GC/ECD	Miller <i>et al.</i> 1984
			22	1.09×10^{-3}	gen. col.-GC/ECD	Opperhuizen <i>et al.</i> 1988
			25	2.27×10^{-4}	gen. col.-GC/ECD	Dunnivant & Elzerman 1988
			25	3.29×10^{-3}	gen. col.-GC/ECD	Li <i>et al.</i> 1992
			25	3.32×10^{-3}	gen. col.-GC/ECD	Li & Doucette 1993
			25	2.84×10^{-3}	gen. col.-GC/ECD	Li & Andren 1994
			25	3.40×10^{-3}	gen. col.-GC/ECD	van Haelst <i>et al.</i> 1996
			5	1.00×10^{-3}	gen. col.-GC/ECD	Shiu <i>et al.</i> 1997
50.7	25–50 °C	Dickhut <i>et al.</i> 1986	15	1.70×10^{-3}		
			25	2.80×10^{-3}		
			35	4.30×10^{-3}		
			45	6.40×10^{-3}		
			recommended value at 25 °C: $(3.0 \pm 0.30) \times 10^{-3} \text{ g}\cdot\text{m}^{-3}$			
			25	1.80×10^{-4}	gen. col.-GC/ECD	Weil <i>et al.</i> 1974
			25	3.90×10^{-4}	gen. col.-GC/ECD	Miller <i>et al.</i> 1984
			20	1.29×10^{-4}	gen.col.-GC/ECD	Dickhut <i>et al.</i> 1986
			25	1.29×10^{-4}		
			$S/(\text{mol/L}) = 6.91 \times 10^{-11} \cdot \exp(0.064 \cdot t)$			
50.6	25–59 °C	Doucette & Andren 1988	recommended value at 25 °C: $(1.50 \pm 0.3) \times 10^{-3} \text{ g}\cdot\text{m}^{-3}$			
			32	2.15×10^{-4}		
			50	7.73×10^{-4}		
			$S/(\text{mol/L}) = 6.91 \times 10^{-11} \cdot \exp(0.064 \cdot t)$			
			25	2.55×10^{-5}	gen. col.-GC/ECD	Dickhut <i>et al.</i> 1986
			32	5.11×10^{-5}		
			40	6.59×10^{-5}		
			50	1.39×10^{-4}		
			$S/(\text{mol/L}) = 1.27 \times 10^{-11} \cdot \exp(0.062 \cdot t)$			
			22	7.82×10^{-5}	gen. col.-GC/ECD	Opperhuizen <i>et al.</i> 1988
49.8	25–50 °C	Dickhut <i>et al.</i> 1986	recommended value at 25 °C:			
			25	1.60×10^{-5}	gen. col.-GC/ECD	Weil <i>et al.</i> 1974
			32	7.50×10^{-6}	gen. col.-GC/ECD	Miller <i>et al.</i> 1984
			40	6.48×10^{-7}	gen. col.-GC/ECD	Dickhut <i>et al.</i> 1986
66.6	40–80 °C	Doucette & Andren 1988	$S/(\text{mol/L}) = 1.27 \times 10^{-11} \cdot \exp(0.062 \cdot t)$			
			25	1.60×10^{-5}	gen. col.-GC/ECD	Weil <i>et al.</i> 1974
			32	7.50×10^{-6}	gen. col.-GC/ECD	Miller <i>et al.</i> 1984
			40	6.48×10^{-7}	gen. col.-GC/ECD	Dickhut <i>et al.</i> 1986

TABLE 2. Aqueous solubilities and reported equations of chlorobenzenes, chlorinated dioxins and dibenzofurans—Continued

Compound			<i>t</i> /°C	Solubility (g/m ³)	Method	Reference
decachlorobiphenyl (cont'd)						
66.6	40–80 °C	Doucette & Andren 1988	60	8.38×10 ⁻⁶		
			70	1.76×10 ⁻⁵		
			80	4.95×10 ⁻⁵		
			<i>S</i> /(mol/L)=1.80×10 ⁻¹³ ·exp(0.077· <i>t</i>)			
			22	2.10×10 ⁻⁵	gen. col.-GC/ECD	Opperhuizen <i>et al.</i> 1988
			recommended value at 25 °C: 1.0×10 ⁻⁶ g·m ⁻³			
Dioxins:						
dibenzo- <i>p</i> -dioxin			4.1	0.212	gen. col.-GC/ECD	Doucette & Andren 1988
$\Delta_{\text{sol}}H/\text{kJ}\cdot\text{mol}^{-1}$			25	0.8998		
48.6	4–32 °C	Doucette & Andren 1988	40	2.392		
50.68	5–45 °C	Shiu <i>et al.</i> 1988	<i>S</i> /(mol/L)=8.85×10 ⁻⁷ ·exp(0.067· <i>t</i>)			
			5	0.205	gen. col.-HPLC/UV	Shiu <i>et al.</i> 1988
			15	0.46		
			25	0.842		
			35	1.762		
			45	3.262		
			recommended value at 25 °C: 0.85±0.05 g·m ⁻³			
1-chloro-			5	0.136	gen. col.-HPLC/UV	Shiu <i>et al.</i> 1988
$\Delta_{\text{sol}}H/\text{kJ}\cdot\text{mol}^{-1}$			15	0.233		
40.85	5–45 °C	Shiu <i>et al.</i> 1988	25	0.417		
			35	0.725		
			45	1.24		
			recommended value at 25 °C: 0.42±0.02 g·m ⁻³			
2-chloro-			3.9	0.1333	gen. col.-GC/ECD	Doucette & Andren 1988
$\Delta_{\text{sol}}H/\text{kJ}\cdot\text{mol}^{-1}$			25	0.3190		
34.0	4–32 °C	Doucette & Andren 1988	39	0.7495		
53.55	5–45 °C	Shiu <i>et al.</i> 1988	<i>S</i> /(mol/L)=4.88×10 ⁻⁷ ·exp(0.048· <i>t</i>)			
			5	0.0635	gen. col.-HPLC/UV	Shiu <i>et al.</i> 1988
			15	0.137		
			25	0.278		
			35	0.653		
			45	1.109		
			recommended value at 25 °C: 0.30±0.02 g·m ⁻³			
2,3-dichloro-			5	0.003 68	gen. col.-HPLC/UV	Shiu <i>et al.</i> 1988
$\Delta_{\text{sol}}H/\text{kJ}\cdot\text{mol}^{-1}$			15	0.007 16		
51.3	5–45 °C	Shiu <i>et al.</i> 1988	25	0.0149		
			35	0.0304		
			45	0.0586		
			recommended value at 25 °C: 0.015±0.003 g·m ⁻³			
2,7-dichloro-			5	0.001 09	gen. col.-HPLC/UV	Shiu <i>et al.</i> 1988
$\Delta_{\text{sol}}H/\text{kJ}\cdot\text{mol}^{-1}$			15	0.002 01		
46.32	5–45 °C	Shiu <i>et al.</i> 1988	25	0.003 75		
			35	0.007 27		
			45	0.0134		
			25	2.24×10 ⁻³	gen. col.-GC/MS	Santl <i>et al.</i> 1994
			recommended value at 25 °C: 0.003 75±0.0005 g·m ⁻³			
2,8-dichloro-			5	0.004 42	gen. col.-HPLC/UV	Shiu <i>et al.</i> 1988
$\Delta_{\text{sol}}H/\text{kJ}\cdot\text{mol}^{-1}$			15	0.008 59		
50.04	5–45 °C	Shiu <i>et al.</i> 1988	25	0.016 74		
			35	0.027 53		
			45	0.0515		
			recommended value at 25 °C: 0.017±0.005 g·m ⁻³			
1,2,4-trichloro-			5	0.002 19	gen. col.-HPLC/UV	Shiu <i>et al.</i> 1988
$\Delta_{\text{sol}}H/\text{kJ}\cdot\text{mol}^{-1}$			15	0.004 77		
46.62	5–45 °C	Shiu <i>et al.</i> 1988	25	0.008 41		
			35	0.016 68		
			45	0.028 22		
			25	0.006 95	gen. col.-GC/MS	Santl <i>et al.</i> 1994
			recommended value at 25 °C: 0.008 41 g·m ⁻³			

TABLE 2. Aqueous solubilities and reported equations of chlorobenzenes, chlorinated dioxins and dibenzofurans—Continued

Compound			<i>t</i> /°C	Solubility (g/m ³)	Method	Reference
1,2,3,4-tetrachloro- $\Delta_{\text{sol}}H/\text{kJ}\cdot\text{mol}^{-1}$			4	1.13×10^{-4}		
			25	4.70×10^{-4}	gen. col.-GC/ECD	Doucette & Andren 1988
46.8	4–40 °C	Doucette & Andren 1988	40	1.17×10^{-3}		
46.86	4–40 °C	Lodge 1989		$S/(\text{mol/L}) = 2.75 \times 10^{-10} \cdot \exp(0.065 \cdot t)$		
33.36	5–45 °C	Shiu <i>et al.</i> 1988	5	0.000 343	gen. col.-HPLC/UV	Shiu <i>et al.</i> 1988
			15	0.000 45		
			25	0.000 63		
			35	0.001 14		
			45	0.002 085		
			25	0.000 388	gen. col.-GC/MS	Santl <i>et al.</i> 1994
				recommended value at 25 °C: $(5.5 \pm 1.0) \times 10^{-4} \text{ g}\cdot\text{m}^{-3}$		
1,2,3,7-TCDD $\Delta_{\text{sol}}H/\text{kJ}\cdot\text{mol}^{-1}$			20	4.30×10^{-4}	gen. col.-HPLC/LSC	Webster <i>et al.</i> 1985
			40	1.27×10^{-3}		
41.84	20–40 °C	Lodge 1989	20	4.30×10^{-4}	gen. col.-HPLC/LSC	Friesen <i>et al.</i> 1985
39.8	7–41 °C	Friesen & Webster 1990	40	1.27×10^{-3}		
			7	8.00×10^{-4}	gen. col.-HPLC/LSC	Friesen & Webster 1990
			11.5	8.00×10^{-4}		
			17	1.30×10^{-3}		
			21	1.50×10^{-3}		
			26	2.30×10^{-3}		
			41	4.30×10^{-3}		
				recommended value at 25 °C: 0.000 42 g·m ⁻³		
1,3,6,8-TCDD $\Delta_{\text{sol}}H/\text{kJ}\cdot\text{mol}^{-1}$			20	3.20×10^{-4}	gen. col.-HPLC/LSC	Webster <i>et al.</i> 1985
			40	3.90×10^{-4}		
8.368	20–40 °C	Lodge 1989	20	3.20×10^{-4}	gen. col.-HPLC/LSC	Friesen <i>et al.</i> 1985
			40	3.90×10^{-4}		
				recommended value at 25 °C: 0.000 32 g·m ⁻³		
2,3,7,8-TCDD $\Delta_{\text{sol}}H/\text{kJ}\cdot\text{mol}^{-1}$			25	2.00×10^{-4}	shake flask-GC/ECD	Crummett & Stehl 1973
			25	3.17×10^{-4}	gen. col.-HPLC/LSC	Webster <i>et al.</i> 1985
188.28	4–17 °C	Lodge 1989	22	1.93×10^{-5}	thin film-LSC	Marple <i>et al.</i> 1986
			22	1.25×10^{-5}	thin film-GC/LRMS	
			25	7.91×10^{-7}	shake flask-LSC	Adams & Blaine 1986
			4.3	1.29×10^{-5}	gen. col.-GC/ECD	Lodge 1989
			17.3	4.83×10^{-4}		
				recommended value at 25 °C: $1.93 \times 10^{-5} \text{ g}\cdot\text{m}^{-3}$		
1,2,3,4,7-PCDD $\Delta_{\text{sol}}H/\text{kJ}\cdot\text{mol}^{-1}$			20	1.20×10^{-4}	gen. col.-HPLC/LSC	Friesen <i>et al.</i> 1985
			40	4.60×10^{-4}		
47.5	7–41 °C	Friesen & Webster 1990	7	1.42×10^{-4}	gen. col.-HPLC/LSC	Friesen & Webster 1990
			11.5	1.88×10^{-4}		
			17	2.44×10^{-4}		
			21	3.45×10^{-4}		
			26	4.63×10^{-4}		
			41	1.28×10^{-3}		
				recommended value at 25 °C: $1.18 \times 10^{-4} \text{ g}\cdot\text{m}^{-3}$		
1,2,3,4,7,8-H ₆ CDD $\Delta_{\text{sol}}H/\text{kJ}\cdot\text{mol}^{-1}$			20	4.40×10^{-6}	gen. col.-HPLC/LSC	Friesen <i>et al.</i> 1985
			40	1.90×10^{-5}		
45.5	7–41 °C	Friesen & Webster 1990	7	5.91×10^{-6}	gen. col.-HPLC/LSC	Friesen & Webster 1990
			11.5	7.98×10^{-6}		
			17	1.07×10^{-5}		
			21	1.25×10^{-5}		
			26	2.02×10^{-5}		
			41	4.86×10^{-5}		
				recommended value at 25 °C: $4.42 \times 10^{-6} \text{ g}\cdot\text{m}^{-3}$		
1,2,3,4,6,7,8-H ₇ CDD $\Delta_{\text{sol}}H/\text{kJ}\cdot\text{mol}^{-1}$			20	2.40×10^{-5}	gen. col.-HPLC/LSC	Friesen <i>et al.</i> 1985
			40	6.30×10^{-6}		
42.4	7–41 °C	Friesen & Webster 1990	7	2.20×10^{-6}	gen. col.-HPLC/LSC	Friesen & Webster 1990
			11	2.69×10^{-6}		
			17	3.04×10^{-6}		
			21	5.40×10^{-6}		
			26	6.03×10^{-6}		
			41	1.49×10^{-5}		

TABLE 2. Aqueous solubilities and reported equations of chlorobenzenes, chlorinated dioxins and dibenzofurans—Continued

Compound		<i>t</i> /°C	Solubility (g/m ³)	Method	Reference
octachloro- $\Delta_{\text{sol}}H/\text{kJ}\cdot\text{mol}^{-1}$ 74.5	40–80 °C Doucette & Andren 1988	20	4.00×10^{-7}	gen. col.-HPLC/LSC	Webster <i>et al.</i> 1985
		40	2.00×10^{-6}		
		20	4.00×10^{-7}	gen. col.-HPLC/LSC	Friesen <i>et al.</i> 1985
		40	2.00×10^{-6}		
		40	3.11×10^{-7}	gen. col.-GC/ECD	Doucette & Andren 1988
		60	1.82×10^{-6}		
		80	7.87×10^{-6}		
		$S/(\text{mol/L}) = 2.77 \times 10^{-14} \cdot \exp(0.081 \cdot t)$			
		recommended value at 25 °C: $7.4 \times 10^{-8} \text{ g}\cdot\text{m}^{-3}$			
Dibenzofurans:					
dibenzofuran $\Delta_{\text{sol}}H/\text{kJ}\cdot\text{mol}^{-1}$ 29.8	4–32 °C Doucette & Andren 1988	25	10.02	shake flask-HPLC	Banerjee <i>et al.</i> 1980
		4	1.652	gen. col.-GC/ECD	Doucette & Andren 1988
33.3	5–45 °C Shiu <i>et al.</i> 1997	25	4.222		
		39.8	6.963		
		$S/(\text{mol/L}) = 8.32 \times 10^{-6} \cdot \exp(0.041 \cdot t)$			
		5	1.914	gen.col.-HPLC/UV	Shiu <i>et al.</i> 1997
		15	3.004		
		25	4.75		
		35	7.56		
		45	11.7		
		25	4.69	shake flask-HPLC/UV	Shiu <i>et al.</i> 1997
		recommended value at 25 °C: $4.75 \pm 0.20 \text{ g}\cdot\text{m}^{-3}$			
2,8-dichloro $\Delta_{\text{sol}}H/\text{kJ}\cdot\text{mol}^{-1}$ 44.9	4–32 °C Doucette & Andren 1988	4.5	0.00384	gen. col.-GC/ECD	Doucette & Andren 1988
		25	0.0145		
2,3,7,8-TCDF 2,3,4,7,8-PCDF 1,2,3,4,7,8-H6CDF 1,2,3,6,7,8-H6CDF 1,2,3,4,6,7,8-H7CDF octachloro- $\Delta_{\text{sol}}H/\text{kJ}\cdot\text{mol}^{-1}$ 62.5	40–80 °C Doucette & Andren 1988	39.5	0.0339		
		$S/(\text{mol/L}) = 1.24 \times 10^{-8} \cdot \exp(0.062 \cdot t)$			
		recommended value at 25 °C: $0.0145 \text{ g}\cdot\text{m}^{-3}$			
		22.7	4.19×10^{-4}	gen. col.-GC/MS	Friesen <i>et al.</i> 1990
		22.7	2.16×10^{-4}	gen. col.-GC/MS	Friesen <i>et al.</i> 1990
		22.7	8.25×10^{-6}	gen. col.-GC/MS	Friesen <i>et al.</i> 1990
		22.7	1.77×10^{-5}	gen. col.-GC/MS	Friesen <i>et al.</i> 1990
		22.7	1.35×10^{-6}	gen. col.-GC/MS	Friesen <i>et al.</i> 1990
		39.5	3.85×10^{-6}	gen. col.-GC/ECD	Doucette & Andren 1988
		58.6	1.40×10^{-5}		
62.5	40–80 °C Doucette & Andren 1988	80	5.86×10^{-5}		
		$S/(\text{mol/L}) = 6.87 \times 10^{-14} \cdot \exp(0.068 \cdot t)$			
		25	1.16×10^{-6}		Doucette & Andren 1988
		recommended value at 25 °C: $1.16 \times 10^{-6} \text{ g}\cdot\text{m}^{-3}$			

Note:

S-solubility in $\text{g}\cdot\text{m}^{-3}$, $\text{mg}\cdot\text{L}^{-1}$; or $\mu\text{g}\cdot\text{kg}^{-1}$; c in $\text{mol}\cdot\text{m}^{-3}$; x is mole fraction.

T - temperature in K; t in °C; θ in K.

R - gas constant.

IR - infrared spectroscopy,

UV - UV spectrophotometry,

GC - gas chromatography,

fluo. - fluorescence spectrophotometry,

GC/FID - GC analysis with flame ionization detector,

GC/ECD - GC analysis with electron capture detector,

GC/MS - GC mass spectrometry,

HPLC - high pressure liquid chromatography,

HPLC/UV - HPLC analysis with UV detector,

HPLC/fluo. - HPLC analysis with fluorescence detector,

gen. col. - generator (or saturation) column technique for preparation of saturated aqueous solution,

SPME - solid phase microextraction technique,

 $\Delta_{\text{sol}}H$ - enthalpy of solution.

TABLE 3. Vapor pressures and reported equations of chlorobenzenes, chlorinated dioxins and dibenzofurans, t in °C and T in K

Compounds	$t/^\circ\text{C}$ or temp range	$-20\text{--}30$	$\log p/\text{mmHg}=7.532-1949.5/T$	Method	Reference
chlorobenzene					Zil'berman-Granovskaya & Shugam 1940
	-13	133.32	-13-133.2 °C	compiled, evaluated data	Stull 1947
	10.6	666.61			
	22.2	1333			
	35.3	2666			
	49.7	5333			
	58.3	7999			
	70.7	13.332			
	89.4	26.664			
	110	53.329			
	132.2	101.325			
	62-131	$\log p/\text{mmHg}=7.18473-1556.6/(t+230)$		Antoine eq. from exptl. data boiling point measurement	Dreisbach & Martin 1949
	56.28	7605			Dreisbach & Shrader 1949
	63.05	10.114			
	75.22	16.500			
	101.85	42.066			
	117.3	67.661			
	131.7	101.325			
	62.00	9660			
	66.38	11.558			
	74.13	15.720			
	89.06	27.246			
	98.79	37.961			
	121.1	68.774			
	131.7	101.263			
	25	1567		Antoine eq. calcd from exptl data	Brown 1952
	-13-349.9	$\log p/\text{mmHg}=(-0.2185\times 9067.7/77)+7.717535$		Antoine eq.	Dreisbach 1955
	62-131	$\log p/\text{mmHg}=6.97808-1431.053/(217.550+t)$		from Brown 1952 data	Weast 1972-73
	56.2-131.7	$\log p/\text{Pa}=6.07963-1419.045/(216.633+t)$		from Dreisbach & S 49 data	Boublik <i>et al.</i> 1973
	62-131.7	$\log p/\text{Pa}=6.10416-1431.813/(217.655+t)$		from Brown 1952 data	Boublik <i>et al.</i> 1984
	62-131.7	$\log p/\text{mmHg}=6.97808-1431.05/(t+217.55)$		Antoine eq.	Boublik <i>et al.</i> 1984
	60-132	$\log p/\text{kPa}=6.11512-1438.86/(-54.72+t)$		Antoine eq.	Dean 1985
	132-325	$\log p/\text{kPa}=6.63988-1897.41/(5.21+t)$		Antoine eq.	Stephenson & Malanowski 1987
	-14.2	66.9	-14.2-40 °C	gas saturation	Stephenson & Malanowski 1987
	-5	167			Liu & Dickhut 1994
	10	501			
	25	1410			
	40	3270			
	-15-40	$\ln p/\text{Pa}=-(35.807-11.208 \cdot n_{\text{Cl}})/RT+(22.87+2.302 \cdot n_{\text{Cl}})$			
		n_{Cl} is numbers of chlorine. R is gas constant recommended value at 25 °C: 1580±30 Pa			
	20	133.32	20-179 °C	compiled, evaluated data	Stull 1947
	46	666.61			
	59.1	1333			
	73.4	2666			
1,2-dichlorobenzene					

TABLE 3. Vapor pressures and reported equations of chlorobcnzenes, chlorinated dioxins, and dibenzofurans, t in °C and T in K—Continued

Compounds	t /°C or temp range	p /Pa	Method	Reference
1,2-DCB (cont'd)				
	89.4	5333		
	99.5	7999		
	112.9	13 332		
	133.4	26 664		
	155.8	53 329		
	179	$\log p/\text{mmHg} = 7.32585 - 1824.6/(t + 230)$		Dreisbach & Martin 1949
	87.02	101325		Dreisbach & Shrader 1949
	97.66	5010		
	104.94	7605		
	118.32	10 114		
	147.6	16 500		
	164.65	42 066		
	180.48	67 661		
	25	101325		
	130.82	171		
	154.83	25 234		Dreisbach 1955
	178.66	51 778		McDonald <i>et al.</i> 1959
	179.54	96 998		
	180.54	99 614		
	181.62	101 655		
	20–179	$\log p/\text{mmHg} = -0.2185 \times 109.43 / 0.07T + 8.185275$		Weast 1972–73
	27.8	224.8		Grayson & Fosbray 1982
	32	282.75		
	41.5	59.28		
	48.6	780.14		
	56.3	1252.94		
	61.1	1644.65		
	70	2635.96		
	20	132		
	27.8–70	$\log p/\text{Pa} = 25.4 - 6013/T$		gas saturation-GC, Antoine eq.
	87–180.5	$\log p/\text{Pa} = 6.13305 - 1699.034/(206.944 + t)$		Grayson & Fosbray 1982
	130.8–181.6	$\log p/\text{Pa} = 6.28861 - 1704.435/(219.409 + t)$		Dreisbach & Shrader 1949 data
	131–181	$\log p/\text{mmHg} = 7.14378 - 1407.49/(t + 219.42)$		McDonald <i>et al.</i> 1959 data
	25	265.5		Antoine eq.
	12.6–172	$\log p/\text{Pa} = 11.06745 - 2577.02/T$		gas saturation-GC, interpolated
	100–180	$\log p/\text{kPa} = 6.25918 - 1705.55(-53.56 + T)$		regression from graph
	-14.2	7.73		Antoine eq.
	-5.0	14.7		gas saturation-GC,
	10	56.1		Liu & Dickhut 1994
	25	164		
	40	448		
	-15–40	$\ln p/\text{Pa} = -(35.807 - 11.208 \cdot n_{\text{Cl}})RT + (22.87 + 2.302 \cdot n_{\text{Cl}})$		where n_{Cl} is number of chlorine, R the gas constant
	-16.65	7.056		-17–149 °C
	-9.75	13.20		pressure gauges,

TABLE 3. Vapor pressures and reported equations of chlorobenzenes, chlorinated dioxins and dibenzofurans, t in °C and T in K—Continued

Compounds	t /°C or temp range	p /Pa	Method	Reference
1,2-DCB (cont'd)				
	0.3	30.82		
	10.3	67.09		
	20.35	137.3		
	30.25	264.4		
	40.25	485.5		
	50.15	848.7		
	60.15	1442.0		
	70.05	2313.0		
	80.05	3660.0		
	89.95	5607.0		
	98.79	8103.0		
	— 16.7–14	$p/\text{Pa} = \exp[21.5929 - 4053.86/(T - 50.2358)]$	pressure gauge, Antoine eq.	Polednicek <i>et al.</i> 1996
		recommended value at 25 °C: $170 \pm 20 \text{ Pa}$	compiled, evaluated data	Stull 1947
1,3-dichlorobenzene	12.1	133.32	12.1–173 °C	
	39	667		
	52.9	1333		
	66.2	2666		
	82	5333		
	92.2	7999		
	105	13322		
	125.9	26664		
	149	53330		
	173	101325		
		$\log(p/\text{mmHg}) = 7.30364 + 1782.4(t + 230)$	Antoine eq. boiling point measurement	Dreisbach & Martin 1949 Dreisbach & Shrader 1949
	90.72	7605		
	98.05	10114		
	111.49	16500		
	140.49	42006		
	157.37	67660		
	173	101325		
	25	252	calcd by formula	Dreisbach 1955 West 1972–73
	12.1–173	$\log(p/\text{mmHg}) = (-0.2185 \times 10446.8/T) + 8.017555$	Antoine eq.	
	90.7–173	$\log(p/\text{Pa}) = 6.18083 - 1611.121/(213.817 + t)$	from Dreisbach & Shrader data	Boublik <i>et al.</i> 1984
	91–173	$\log p/\text{mmHg} = 7.0401 - 1607.05/(t + 213.38)$	Antoine eq.	Dean 1985
	25	179.3	gas saturation, interpolated	Rordorf 1985
	12.6–172	$\log p/\text{Pa} = 11.0542 - 2624.11/T$	regression from graph	Rordorf 1985
	67–240	$\log p/\text{KPa} = 6.00535 - 1496.2/(- 72.15 + T)$	Antoine eq.	Stephenson & Malanowski 1987
	—23.55	5.459	pressure gauge	Polednicek <i>et al.</i> 1996
	—19.57	7.99		
	—9.7	19.355		
	0.3	44.17		
	10.34	94.45		
	20.39	190.4		
	30.28	360		
	40.26	652.8		
	50.15	1125		

TABLE 3. Vapor pressures and reported equations of chlorobenzenes, chlorinated dioxins and dibenzofurans, t in °C and T in K—Continued

Compounds	$t^{\circ}\text{C}$ or temp range	p/Pa	Method	Reference
1,3-DCB (cont'd)				
	60.18	1873		
	70.03	2980		
	80	4662		
	89.95	7043		
	98.86	10 180		
	-23.2-1	$p/\text{Pa} = \exp[21.6433 - 4031.27/(T - 47.5846)]$		Polednicek <i>et al.</i> 1996
		recommended value at 25 °C: $260 \pm 40 \text{ Pa}$		
		$\log p/\text{mmHg} = 7.532 - 1949.5/T$		
1,4-dichlorobenzene	20-30			
	54.8	1333	54.8-173.9 °C	compiled and evaluated data
	69.2	2666		
	84.8	5333		
	95.2	7999		
	108.4	13 332		
	128.3	26 664		
	150.2	53 330		
	173.9	101 325		
		$\log p/\text{mmHg} = 7.30697 - 1788.7/(t + 230)$		
	91.998	7605	92-174.1 °C	Antoine eq. boiling point measurement
	99.41	10 114		
	112.66	16 500		
	141.65	42 066		
	158.52	67 660		
	174.12	101 325		
	25	234.5	calcd by formula	Dreisbach 1955
	94.8	8514		McDonald <i>et al.</i> 1959
	98.55	9844		
	104.81	12 444		
	116.28	18 808		
	143.52	44 465		
	159.79	70 117		
	171.87	95 945		
	174.04	101 325		
	30-50	$\log p/\text{mmHg} = (-0.2185 \times 17260.5/T) + 12.4890;$		Weast 1972-73
	54.8-173.9	$\log p/\text{mmHg} = (-0.2185 \times 10611.0/T) + 8.073632;$		Weast 1972-73
	1.47	14.14		de Kruif <i>et al.</i> 1981
	3.94	18 32		
	6.45	23 67		
	8.43	28 88		
	10.33	34 83		
	12.35	42 44		
	14.3	51 13		
	16.63	63 79		
	19.84	85.98		
	1.47-20	$R \cdot \ln p/\text{Pa} = -8543/284.15 + 65700(1/284.15 - 1/T)$		de Kruif <i>et al.</i> 1981
	92-174	$\log p/\text{Pa} = 6.12531 - 1576.471/(208.538 + t)$		Boublik <i>et al.</i> 1984
			from Dreisbach & Shrader data	

TABLE 3. Vapor pressures and reported equations of chlorobenzenes, chlorinated dioxins and dibenzofurans, t in °C and T in K—Continued

Compounds	$t/^\circ\text{C}$ or temp range	p/Pa	Method	Reference
1,4-nDCB (cont'd)	95–174 95–174	$\log p/\text{Pa} = 6.140\,44 \cdots 1587\,243 / (209\,829 + t)$ $\log p/\text{mmHg} = 7.0208 \cdots 1590.9 / (t + 210.2)$	from McDonald <i>et al.</i> 59 data Antoine eq. gas saturation gas saturation-GC, solid	Boublik <i>et al.</i> 1984 Dean 1985 Chiou & Shoup 1985 Rordorf 1985
	20	86.7		
	25	158		
	50	1218		
	75	6993		
	100	31774		
	125	119380		
	150	383590		
	~30–47	$\log p/\text{Pa} = 13.874 - 3450/T$	regression from graph, solid	Rordorf 1985
	20–40	$\log p/\text{kPa} = 10.472 - 3382.9/T$	Antoine eq. for solid	Stephenson & Malanowski 1987
	37–53	$\log p/\text{kPa} = 10.181 - 3290.4/T$	Antoine eq., solid	
	68–175	$\log p/\text{kPa} = 6.126\,95 - 1578.51 / (-64.22 + T)$	Antoine eq. for liquid	
	-14.5	4.67	gas saturation-GC	Liu & Dickhut 1994
	-5.0	16.0		
	10	31.7		
	25	133		
	40	452		
	-15–40	$\ln p/\text{Pa} = -(35.807 - 11.208 \cdot n_{\text{Cl}}) / \text{RT} + (22.87 + 2.302 \cdot n_{\text{Cl}}); n_{\text{Cl}}$ is no. of Cl pressure gauges, solid		Liu & Dickhut 1994
	0.34	12.2		
	10.35	34.25		
	20.35	88.7		
	30.31	215		
	40.25	485.5		
	50.15	1037		
	0.34–50.16	$p/\text{Pa} = \exp[21.0472 - 3665.96 / (T - 62.3849)]$	pressure gauge, Antoine eq. pressure gauges, liquid	Polednicek <i>et al.</i> 1996
	60.22	1840		
	70.03	2948		
	80.03	4630		
	89.95	7040		
	98.75	9904		
	108.65	14342		
	118.65	20385		
	128.75	28345		
	60.15–168.9	$p/\text{Pa} = \exp[28.4986 - 6272.86 / (T - 32.2741)]$	pressure gauge, Antoine eq.	Polednicek <i>et al.</i> 1996
1,2,3-trichlorobenzene	recommended value at 25 °C: $130 \pm 20 \text{ Pa}$		compiled, evaluated data, solid compiled, evaluated data, liquid	Still 1947
	40	133.3		
	70	666.6		
	85.5	1333		
	101.8	2666		
	119.8	5333		
	131.5	7999		
	146	13332		
	168.2	26664		
	193.5	53330		
	218.5	101325		

TABLE 3. Vapor pressures and reported equations of chlorobenzenes, chlorinated dioxins and dibenzofurans, t in °C and T in K—Continued

Compounds	$t^{\circ}\text{C}$, or temp range	p/Pa	Method	Reference
1,2,3-TCB (cont'd)	16–30 °C 40–218.5	$\log p/\mu\text{m} = -3340.2/T + 13.662$ $\log p/\text{mmHg} = -0.2185 \times 11.349.5/T + 7.916468$	Rodebush gauge, Antoine eq.	Sears & Hopke 1949b
	25	25.09	Antoine eq.	Weast 1972–73
	~30–60	$\log p/\text{Pa} = 14.3125 - 3850/T$, solid	gas saturation, interpolated	Rordorf 1985
	16–30	$\log p/\text{kPa} = 9.787 - 3440/T$	regression eq., from graph	Rordorf 1985
	70–219	$\log p/\text{kPa} = 7.230.08 - 2624.09/(10.506 + T)$	Antoine eq., solid	Stephenson & Malanowski 1987
	–15	0.124	Antoine eq., liquid	Liu & Dickhut 1994
	5.0	0.445	gas saturation-GC	
	10	2.80		
	25	11.20		
	40	50.50		
	–15–40	$\ln p/\text{Pa} = -(35.807 - 11.208 \cdot n_{\text{Cl}}/\text{RT}) + (22.87 + 2.302 \cdot n_{\text{Cl}})$; n_{Cl} is no. of Cl	pressure gauges, solid	Liu & Dickhut 1994
	0.36	0.95	pressure gauges, solid	Polednick et al. 1996
	10.55	2.97		
	20.35	8.82		
	30.28	23.64		
	50.12	146		
	60.11	$p/\text{Pa} = \exp[21.1681 - 4077.21/(T - 71.5639)]$	pressure gauge, Antoine eq.	Polednick et al. 1996
	70.03	268.14	pressure gauge, liquid	Polednick et al. 1996
	80.01	472.25		
	88.73	799		
	98.03	1240		
	108.67	1306		
	118.69	3055		
	128.73	4618		
	60.1–169	6805		
		$p/\text{Pa} = \exp[33.2977 - 9325.37/(T - 6.13455)]$	pressure gauge, Antoine eq.	Polednick et al. 1996
	recommended value at 25 °C: $15 \pm 5 \text{ Pa}$	133.32	compiled, evaluated data, liquid	
	38.4	666.61		
	67.3	1333		
	81.7	2666		
	97.2	5333		
	114.8	7999		
	125.7	13.332		
	140	26.664		
	162	53.330		
	187.7	101.325		
	213	101.325		
	6–25	$\log p_s/\mu\text{m} = -3254.0/T + 13.445$	Rodebush gauge, Antoine eq., solid	Sears & Hopke 1949b
	6–25	$\log p_L/\mu\text{m} = -2452.3/T + 10.682$	Rodebush gauge, Antoine eq., liquid	Sears & Hopke 1949b
	25	38.76	calc'd from formula	Dreisbach 1955
	38.4–213	$\log p/\text{mmHg} = (-0.2185 \times 11425.1/T) + 8.030523$	Antoine eq.	Weast 1972–73
	22	26.4	gas saturation-GC	Politzki et al. 1982
	25	28.5	gas saturation, interpolated	Rordorf 1985
	~30–97	$\log p/\text{Pa} = 11.23927 - 2917.37/T$	regression from graph, liq.	Rordorf 1985
	6–17	$\log p/\text{kPa} = 9.570 - 3254/T$	Antoine eq., solid	Stephenson & Malanowski 1987

TABLE 3. Vapor pressures and reported equations of chlorobenzenes, chlorinated dioxins and dibenzofurans, t in °C and T in K—Continued

TABLE 3. Vapor pressures and reported equations of chlorobenzenes, chlorinated dioxins, and dibenzofurans, t in °C and T in K—Continued

Compounds	<i>T</i> /°C or temp range	<i>p</i> /Pa	Method	Reference
1,2,3,4-TeCB (cont'd)				
1,2,3,5-tetrachlorobenzene	68–5254	$\log p/\text{mmHg} = (-0.2185 \times 128.725/T) + 8.251056$	Antoine eq.	Weast 1972–73
	25	4.017, 3.49	GC-RT correlation, supercooled liq.	Bridleman 1984
	25	6.28	gas saturation, extrapolated, solid	Rordorf 1985
	~30–47	$\log p/\text{Pa} = 13.52904 - 3793.25/T$	regression eq. from graph	Rordorf 1985
	47–97	$\log p/\text{Pa} = 11.590 - 3555.42/T$, liquid	regression eq. from graph, liq.	Rordorf 1985
	58–254	$\log p/\text{kPa} = 5.7081 - 1517.2/(T - 117.384)$	Antoine eq., liquid	Stephenson & Malanowski 1987
	25	8.00	GC-RT correlation, supercooled liq.	Hinckley <i>et al.</i> 1990
	recommended value at 25 °C: 5.2±1.0 Pa		compiled, evaluated data	
	58.2	133	58.2–246 °C	Stull 1947
	89	667		
	101.1	1333		
	121.6	2666		
	140	5333		
	152	7999		
	168	13 332		
	193.7	26 664		
	220.5	53 329		
	246	133 323		
	58.2–246	$\log p/\text{mmHg} = (-0.2185 \times 151.24/T) + 8.907497$	Antoine eq.	Weast 1972–73
	25	5.085	gas saturation, extrapolated, solid	Rordorf 1985
	~30–47	$\log p/\text{Pa} = 14.09357 - 3991.42/T$,	regression eq. from graph, solid	Rordorf 1985
	25	5.86	gas saturation, extrapolated, liq.	Rordorf 1985
	~47–97	$\log p/\text{Pa} = 10.9315 - 3030/T$	regression eq. from graph, liq.	Rordorf 1985
	58–246	$\log p/\text{kPa} = 6.7756 - 2394.0/(T - 17.85)$	Antoine eq., liquid	Stephenson & Malanowski 1987
	recommended value at 25 °C: 5.50±0.5 Pa		compiled, evaluated data	
	146	5333	146–245 °C	Stull 1947
	157.7	7999		
	173.5	13 332		
	196	26 664		
	220.5	53 329		
	245	133 323		
	146–245	$\log p/\text{mmHg} = (-0.2185 \times 128.288/T) + 8.282213$	Antoine eq., liquid	Weast 1972–73
	25	~0.02	evaporation rate	Dohbs & Cull 1982
	25	0.924	gas saturation, extrapolated, solid	Rordorf 1985
	~35–110	$\log p/\text{Pa} = 14.3075 - 4290.4/T$	regression eq. from graph, solid	Stephenson & Malanowski 1987
	146–243	$\log p/\text{kPa} = 9.1357 - 4632.36/(132.953 + T)$	Antoine eq., liquid	
	recommended value at 25 °C: 0.72 Pa		compiled, evaluated data	
	98.6	133	98.6–276 °C	Stull 1947
	129.7	667		
	144.3	1333		
	160	2666		
	178.5	5333		
	190.1	7999		
	205.5	13 332		
	227	26 664		
	251.5	53 329		
pentachlorobenzene				

TABLE 3. Vapor pressures and reported equations of chlorobenzenes, chlorinated dioxins and dibenzofurans, t in °C and T in K—Continued

Compounds	$t/^\circ\text{C}$ or temp range	p/Pa	Method	Reference
PCB (cont'd)				
	276	133 323	Antoine eq., liquid	Weast 1972–73
	98.6–276	$\log p/\text{mmHg} = (-0.2185 \times 15124.2/T) + 8.907497$	evaporation rate	Dobbs & Cull 1982
	25	0.055	gas saturation, extrapolated	Rordorf 1985
	25	1.44	regression eq. from graph, solid	
	~30–60	$\log p/\text{Pa} = 15.6714 - 4830.4/T$	Antoine eq., liquid	Stephenson & Malanowski 1987
	98–276	$\log p/\text{kPa} = 8.00795 - 3325.33/(4.814 + T)$	pressure gauge, solid	Polednicek <i>et al.</i> 1996
	30.3	0.39		
	40.27	1.16		
	50.27	3.22		
	60.16	8.48		
	70.05	20.4		
	80.02	47.3		
	0.36–50.12	$p/\text{Pa} = \exp[23.4783 - 6188.33(T - 34.6922)]$	pressure gauge, Antoine eq.	Polednicek <i>et al.</i> 1996
	98.65	168	pressure gauge, liquid	Polednicek <i>et al.</i> 1996
	108.65	285		
	118.82	471		
	128.85	756		
	138.9	1190		
	149.01	1821		
	159.05	2731		
	60.11–169.5	$p/\text{Pa} = \exp[30.4445 - 8654.67/(T - 27.6534)]$	pressure gauge, Antoine eq.	Polednicek <i>et al.</i> 1996
	recommended value at 25 °C: 0.22±Pa			
hexachlorobenzene (HCB)				
	114.4	133	114–309 °C	Stull 1947
	149.3	667	compiled, evaluated data, solid	
	166.4	1333		
	185.7	2666		
	206	5333		
	219	7999		
	235.5	13 332		
	258.5	26 664		
	283.5	53 329		
	309.4	133 323		
	96–124	$\log p/\text{mmHg} = -4793.6/T + 11.397$	Rodebush gauge, Antoine eq.	Sears & Hopke 1949a
	114.4–309	$\log p/\text{mmHg} = (-0.2185 \times 15199.1/T) + 8.550497$	Antoine eq.	Weast 1972–73
	15	0.000 528	gas saturation technique	Farmer <i>et al.</i> 1980
	25	0.002 55		
	35	0.008 53		
	45	0.0279		
	25	0.0023	interpolated from exptl data	
	15–45	$\log p/\text{mmHg} = 12.94 - 5279/T$	gas saturation, Antoine eq.	Farmer <i>et al.</i> 1980
	10	8.00×10^{-4}	gas saturation, solid	OECD 1981
	20	2.60×10^{-3}		
	30	8.10×10^{-3}		
	40	2.30×10^{-2}		
	50	6.10×10^{-2}		
	10	2.80×10^{-4}	10–50 °C	vapor pressure balance method
				OECD 1981

TABLE 3. Vapor pressures and reported equations of chlorobenzenes, chlorinated dioxins and dibenzofurans, t in °C and T in K—Continued

Compounds	t /°C or temp range	p /Pa	Method	Reference
HCB (cont'd)				
20		1.10×10^{-3}		
30		3.00×10^{-3}		
40		1.30×10^{-2}		
50		3.90×10^{-2}		
25		0.0006	evaporation rate	Gückel <i>et al.</i> 1982
		$\log p/\text{mmHg} = 12.237 - 5152.1/T$	evaporation rate, Antoine eq.	
20		0.00046	evaporation rate	Dobbs & Cull 1982
25		0.0002	evaporation rate	Dobbs <i>et al.</i> 1984
25		0.303, 0.121	GC-RT correlation, supercooled liq.	Bidleman 1984
25		0.003 32	gas saturation, extrapolated	Rordorf 1985
~35–95		$\log p/\text{Pa} = 14.9625 - 5200/T$	regression eq. from graph, solid	Rordorf 1986
41.05		0.0205	gas saturation-GC	
50.16		0.0547		
60.3		0.165		
70.3		0.452		
80.3		1.155		
90.4		2.77		
100.25		6.29		
40–100		$\log p/\text{Pa} = [(12.3243 - 4336.95/T)/(1 - 41.1905/T)]$	Antoine eq., solid	Rordorf 1986
114–229		$\log p_S/\text{kPa} = 7.007\ 06 - 2831.85/(T - 28.25)$	Antoine eq., solid	Stephenson & Malanowski 1987
229–316		$\log p_L/\text{kPa} = 7.352\ 48 - 2786.78/(T - 61.33)$	Antoine eq., liquid	Stephenson & Malanowski 1987
25		0.303	GC-RT correlation, supercooled liq.	Hinckley <i>et al.</i> 1990
25		0.127	GC-RT correlation, supercooled liq.	
~15		$\log p_L/\text{Pa} = 11.11 - 3582/T$	Antoine eq., supercooled liq.	Hinckley <i>et al.</i> 1990
~5		2.21×10^{-6}	gas saturation-GC,	Liu & Dickhut 1994
10		2.38×10^{-5}		
25		2.62×10^{-4}		
25		3.11×10^{-3}		
40		0.121		
~15–40		$\ln p/\text{Pa} = -[(35.807 - 11.208 \cdot n_{\text{Cl}})/\text{RT}] + (22.87 + 2.302 \cdot n_{\text{Cl}})$		
~20–30		$\log p/\text{Pa} = 10.83 - 4404/T, \Delta H = 77.4 \text{ kJ/mol}$	gas saturation, Antoine eq.	Liu & Dickhut 1994
~30		2.567×10^{-6}	gas saturation-GC	Wania <i>et al.</i> 1994
~20		7.257×10^{-6}		Wania <i>et al.</i> 1994
~10		3.229×10^{-5}		
0		1.030×10^{-4}		
10		3.556×10^{-4}		
20		1.092×10^{-3}		
30		3.276×10^{-3}		
		recommended value at 25 °C: 0.0023 Pa		
PCBs:				
2-chlorobiphenyl (PCB-1)	89.3	133		
	109.3	667		
	134.7	1333		
	151.2	2666		
	169.9	5333		
	182.1	7999		
		89.3–267.5 °C	complied, evaluated data	Stull 1947

TABLE 3. Vapor pressures and reported equations of chlorobenzenes, chlorinated dioxins and dibenzofurans, t in °C and T in K—Continued

Compounds	$t/^\circ\text{C}$ or temp range	P/Pa	Method	Reference
PCB-1 (cont'd)				
	197	13.332		
	219.6	26.664		
	243.8	53.329		
	267.5	101.325		
	89.3–267.5	$\log p/\text{mmHg} = (-0.2185 \times 13925.7/T) + 8.484\text{-}380$		Weast 1972–73
	137–267	$\log p/\text{mmHg} = 8.306 - 3018/T$		Geidarov <i>et al.</i> 1975
	25	1.12	quartz manometer data	Neeley 1981, 1983
	28	0.762, 1.50	torsion-Knudsen effusion method	Ferro <i>et al.</i> 1983
	33	1.52, 2.36		
	37	2.30, 3.42		
	40	3.05, 4.13		
	46	3.81, 5.17		
	50	4.57, 6.10		
	50	10.3, 17.3		
	50	8.10, 12.8		
	54	6.10, 9.69		
	54	10.9, 19.2		
	59	16.2, 24.8		
	59	15.8, 22.9		
	63	25.6, 36.9		
	68	34.1, 51.1		
	73	44.3, 65.5		
	81	83.5, 115		
	86	120, 163		
	33–77	$\log p/\text{kPa} = 9.99 - 3893/T$	Knudsen effusion data, liquid	Burkhard <i>et al.</i> 1985
	64–110	$\log p/\text{kPa} = 10.98 - 4406/T$	torsion effusion data, liquid	Ferro <i>et al.</i> 1983
	33–110	$\log p/\text{kPa} = 10.48 - 4149/T$	torsion-Knudsen effusion data	Ferro <i>et al.</i> 1983
	25	1.89, 2.56	GC-RT correlation, supercooled liq.	Bidleman 1984
	25	1.53	extrapolated, solid	
	25	2.20	GC-RT correlation, supercooled liq.	
	96–293	$\log p/\text{kPa} = 9.5876 - 5125.76/(T - 135.232)$	Antoine eq., liquid	Foreman & Bidleman 1985
	136–267	$\log p/\text{kPa} = 7.4309 - 3018/T$	Antoine eq., liquid	Stephenson & Malanowski 1987
		$\log p/\text{kPa} = 11.57 - 3466/T$	GC-RT, supercooled liquid	
		recommended value at 25 °C: $1.0 \pm 0.20 \text{ Pa}$	quartz manometer data	Falconer & Bidleman 1994
3-chlorobiphenyl (PCB-2)	179–263	$\log p/\text{mmHg} = 9.037 - 3445/T$		Geidarov <i>et al.</i> 1975
	25	0.613		Neeley 1981, 1983
	37	1.52, 2.43		Ferro <i>et al.</i> 1983
	40	2.29, 3.62		
	46	3.05, 4.12		
	50	3.81, 6.23		
	56	6.33, 8.53		
	59	13.6, 19.1		
	63	15.8, 22.3		
	68	23.4, 29.0		
	73	27.5, 25.6		
	81	47.3, 63.6		
		av. 55.4		

TABLE 3. Vapor pressures and reported equations of chlorobenzenes, chlorinated dioxins and dibenzofurans, t in °C and T in K—Continued

Compounds	t /°C or temp range	p /Pa	Method	Reference
PCB-3 (cont'd)				
	86	63.2, 84.9	av. 74.0	
	37–86	$\log p/\text{Pa} = 8.45 - 34.58/T$	Knudsen effusion data, liquid	Ferro <i>et al.</i> 1983
	68–129	$\log p/\text{Pa} = 8.91 - 33.71/T$	torsion effusion data, liquid	Ferro <i>et al.</i> 1983
	37–129	$\log p/\text{Pa} = 8.68 - 36.14/T$	torsion-Knudsen effusion data	
	25	0.723	extrapolated	Burkhard <i>et al.</i> 1985
	25	0.997	GC-RT correlation, supercooled liq.	Foreman & Bidleman 1985
			GC-RT correlation, supercooled liq.	Falconer & Bidleman 1994
4-chlorobiphenyl (PCB-3)	recommended value at 25 °C: 1.0±0.20 Pa	96–293 °C	compiled and evaluated data	Stull 1947
	96.4	133		
	129.8	667		
	146	1333		
	164	26666		
	183.8	53333		
	196	7999		
	212.5	13332		
	237.8	26664		
	264.5	53329		
	292.9	101325		
	96.4–293	$\log p/\text{mmHg} = (-0.2185 \times 14017.4/T) + 8.300\ 143$	Antoine eq.	Weast 1972–73
	25	0.60		
	33	0.762, 0.697	av. 7.29	Neely 1981
	35	0.762, 0.917	av. 8.40	Ferro <i>et al.</i> 1983
	37	1.52, 0.902	av. 1.21	
	44	2.29, 1.72	av. 2.0	
	50	3.05, 2.85	av. 2.95	
	50	3.05, 3.57	av. 3.31	
	57	5.33, 6.04	av. 5.69	
	63	9.14, 10.4	av. 9.77	
	73	21.3, 1.83	av. 1.98	
	73	21.1, 1.86	av. 15.3	
	26.85	0.407	solid av. torsion-Knudsen effusion	Ferro <i>et al.</i> 1983
	46.85	2.58		
	66.85	13.1		
	74.75	23.2		
	74.75	12.6	liquid av. torsion-Knudsen effusion	
	86.85	27.7		
	106.85	91.5		
	126.85	268		
	33–73	$\log p/\text{Pa} = 9.44 - 3849/T$	Knudsen effusion data, solid	Ferro <i>et al.</i> 1983
	75–136	$\log p/\text{Pa} = 8.28 - 3541/T$	torsion effusion data, liquid	Ferro <i>et al.</i> 1983
	5.2	0.0111	gas saturation-GC	Burkhard <i>et al.</i> 1984
	15	0.0494		
	24.9	0.172		
	25	0.175		
	5.2–25	$\log p/\text{Pa} = 15.188 - 4754/T$	gas saturation, Antoine eq.	Burkhard <i>et al.</i> 1984
	25	0.931	GC-RT correlation, supercooled liq.	Foreman & Bidleman 1985

TABLE 3. Vapor pressures and reported equations of chlorobenzenes, chlorinated dioxins and dibenzofurans, t in °C and T in K—Continued

Compounds	t /°C or temp range	P /Pa	Method	Reference
PCB-3 (cont'd)	96–293 178–263 –20 –10 0 10 20 30 –20–30	$\log p/\text{kPa} = 7.1989 - 2868.98/(T - 11,566)$ $\log p/\text{kPa} = 8.1619 - 3445/T$ 2.446×10^{-4} 1.297×10^{-3} 4.889×10^{-3} 1.883×10^{-2} 6.771×10^{-2} 0.2233 $\log p/\text{Pa} = 14.15 - 4493/T$ $\log p/\text{Pa} = 11.67 - 3488/T$ recommended value at 25 °C: 0.26 ± 0.10 Pa	Antoine eq., liquid Antoine eq., liquid gas saturation-GC	Stephenson & Malanowski 1987 Wania <i>et al.</i> 1994
2,2'-dichlorobiphenyl (PCB-4)	37.12 41.42 45.89 50.44 54.92 37.12–54.9 25 25 37–55	$0.616, 0.621$ $1.02, 1.011$ $1.68, 1.67$ $2.84, 2.77$ $4.69, 4.65$ $\log p/\text{nmHg} = 13.857 - 5019/T$ 0.357 0.298 $\log p/\text{kPa} = 12.962 - 5019/T$ recommended value at 25 °C: 0.13 ± 0.2 Pa	Knudsen effusion effusion data	Smith <i>et al.</i> 1964 Neely 1981
3,3'-dichloro- (PCB-11)	25 25 25	0.0267 0.0253 $\log p/\text{nmHg} = 10.68 - 4290/T$ $0.0865, 0.0952$ 0.0258 0.907 $\log p/\text{Pa} = 12.14 - 3936/T$ recommended value at 25 °C: 0.026 ± 0.004 Pa	GC-retention time GC-retention time GC-RT correlation, supercooled liq. GC-RT correlation, supercooled liq. extrapolated exptl data, solid GC-RT correlation, supercooled liq. GC-RT correlation, supercooled liq.	Westcott & Bidleman 1981 Bidleman <i>et al.</i> 1983 Bidleman <i>et al.</i> 1983 Bidleman 1984 Burkhard <i>et al.</i> 1985 Foreman & Bidleman 1985 Falconer & Bidleman 1994
4,4'-dichlorobiphenyl (PCB-15)	29.88 66.58 76.78 87 25 30–87 25 25 50–87 5–45 –10 0 10 20 30	$0.0149, 0.0152$ 0.432 $1.26, 1.27$ $3.55, 3.57$ 0.00263 $\log p/\text{nmHg} = 13.460 - 3416/T$ $0.0713, 0.0837$ 0.0263 $0.072, 0.059, 0.0772$ $\log p/\text{kPa} = 12.585 - 5416/T$ $\log p/\text{nmHg} = 10.20 - 4090/T$ 1.206×10^{-5} 8.303×10^{-5} 4.159×10^{-4} 1.197×10^{-3} 4.475×10^{-3} $\log p/\text{Pa} = 12.18 - 3971/T$	Knudsen effusion extrapolated effusion data Antoine eq. from effusion data GC-RT, supercooled liq. value extrapolated exptl data, solid GC-RT, supercooled liq. value Antoine eq., solid GC-retention data gas saturation, solid GC retention data	Smith <i>et al.</i> 1964 Bidleman 1984 Burkhard <i>et al.</i> 1985 Foreman & Bidleman 1985 Stephenson & Malanowski 1987 Tateya <i>et al.</i> 1988 Wania <i>et al.</i> 1994 Falconer & Bidleman 1994

TABLE 3. Vapor pressures and reported equations of chlorobenzenes, chlorinated dioxins and dibenzofurans, t in °C and T in K—Continued

Compounds	t /°C or temp range	p /Pa	Method	Reference
PCB-15 (cont'd)	-10–30	$\log p/\text{Pa} = 14.10 - 4977/T$ recommended value at 25 °C: 0.005 Pa	gas saturation, Antoine eq.	Wania <i>et al.</i> 1994
2,2',5-trichlorobiphenyl (PCB-18)	25	$0.0776, 0.0833$ $\log p/\text{mmHg} = 10.1 - 4090/T$ $\log p/\text{Pa} = 12.09 - 3935/T$	GC-RT correlation, supercooled liq. GC-retention data	Foreman & Bidleman 1985 Tateya <i>et al.</i> 1988 Falconer & Bidleman 1994
2,4,5-trichlorobiphenyl (PCB-29)	25	recommended value at 25 °C: 0.0443 $0.0453, 0.0464, 0.0493$ $\log p/\text{Pa} = 12.09 - 4077/T$	GC-RT, supercooled liq. value GC-RT, supercooled liq. value GC-RT, supercooled liq. value	Bidleman 1984 Foreman & Bidleman 1985 Falconer & Bidleman 1994
2,4,6-trichlorobiphenyl (PCB-30)	124 163 172 25	recommended value at 25 °C: 0.132 Pa 133 1332 2000 0.031	124–172 °C boiling point measurement extrapolated exptl data GC-RT, supercooled liq. value	Augood <i>et al.</i> 1953 Bidleman 1984
2',3,4-trichloro- (PCB-33)	25 25 25 30 30–40	0.00124 $0.111, 0.135, 0.117$ $\log p/\text{Pa} = 12.02 - 3886/T$ recommended value at 25 °C: 0.038 Pa 0.0133 0.0107 0.0133 0.016	extrapolated exptl data GC-RT, supercooled liq. value GC-RT, supercooled liquid gas saturation-GC GC-retention time gas saturation	Burkhard <i>et al.</i> 1985 Foreman & Bidleman 1985 Falconer & Bidleman 1994
2',3,4,5-tetrachloro- (PCB-34)	25 25 25 30 30–40	0.0103 0.0133 0.016 0.0138 $\log p/\text{mmHg} = 1.09 - 1510/T$ $\log p/\text{Pa} = 1.09 - 4480/T$	gas saturation, Antoine eqn GC-retention time gas saturation gas saturation gas saturation gas saturation	Westcott <i>et al.</i> 1981 Bidleman <i>et al.</i> 1983 Bidleman <i>et al.</i> 1983 Bidleman <i>et al.</i> 1983 Westcott <i>et al.</i> 1981
2,2',3,3'-tetrachloro- (PCB-40)	25 25 25 25 25	0.0103 0.0133 0.016 0.0138 0.0138 $\log p/\text{mmHg} = 10.92 - 4480/T$ $\log p/\text{Pa} = 12.09 - 4075/T$ recommended value at 25 °C: 0.012 ± 0.03 Pa 0.0098 $0.00887, 0.00861, 0.0098$ $\log p/\text{mmHg} = 10.7 - 4510/T$ $\log p/\text{Pa} = 12.32 - 4271/T$	gas saturation data GC-RT correlation, solid GC-RT correlation, supercooled liq. GC-RT correlation, supercooled liq. gas saturation-GC, solid GC-retention time gas saturation	Burkhard <i>et al.</i> 1985 Tateya <i>et al.</i> 1988 Falconer & Bidleman 1994 Bidleman 1984 Foreman & Bidleman 1985 Tateya <i>et al.</i> 1988 Falconer & Bidleman 1994 Neely <i>et al.</i> 1983 Foreman & Bidleman 1985 Falconer & Bidleman 1994
2,2',4,4'-tetrachloro- (PCB-47)	25 25	0.0115 $\log p/\text{Pa} = 12.37 - 4229/T$ recommended value at 25 °C: $0.152, 0.156$	gas saturation-GC, solid GC-RT correlation, supercooled liq. GC-RT correlation, supercooled liq.	Westcott & Bidleman 1981 Westcott & Bidleman 1981
2,2',5,5'-tetrachloro- (PCB-52)	25 25 30	0.0073 2.53×10^{-3} 4.80×10^{-3}	gas saturation-GC, solid GC-retention time gas saturation	

TABLE 3. Vapor pressures and reported equations of chlorobenzenes, chlorinated dioxins and dibenzofurans, t in °C and T in K—Continued

Compounds	t /°C or temp range	p /Pa	Method	Reference
PCB-52 (cont'd)	30–40	$\log p/\text{Torr} = 11.8 - 4920/T$	gas saturation, Antoine eq.	Westcott <i>et al.</i> 1981
	25	0.007 07	GC-retention data	Bidleman <i>et al.</i> 1983
	25	0.002 53	gas saturation-GC	Bidleman <i>et al.</i> 1983
	30	0.0048	gas saturation-GC	
		$\log p/\text{mmHg} = 10.87 - 4510/T$	GC-RT data, supercooled liq.	Bidleman <i>et al.</i> 1983
		$\log p/\text{mmHg} = 11.8 - 4920/T$	gas saturation data	
	25	0.0188, 0.0165	GC-RT, supercooled liq., value	Bidleman 1984
		0.004 97	GC-RT correlation, solid	Burkhard <i>et al.</i> 1985
	25	0.0167, 0.0162	GC-RT, supercooled liq., value	Foreman & Bidleman 1985
5–45	25	0.0104, 0.0088	GC-retention data, supercooled liq.	Tateya <i>et al.</i> 1988
	25	$\log p/\text{Pa} = 11.74 - 4127/T$	GC-RT, supercooled liq., value	Hinckley <i>et al.</i> 1990
		$\log p/\text{Pa} = 12.36 - 4220/T$	GC-RT, supercooled liq.	
		recommended value at 25 °C: 0.0050 Pa	GC-RT, supercooled liquid	Falconer & Bidleman 1994
2,3,4,5-tetrachloro-(PCB-61)	-20	5.298×10^{-7}	gas saturation-GC	
	-10	3.817×10^{-6}		Wania <i>et al.</i> 1994
	0	1.439×10^{-5}		
	10	6.163×10^{-5}		
	20	1.854×10^{-4}		
	-20–20	$\log p/\text{Pa} = 12.10 - 4632/T$	gas saturation, Antoine eqn	
		recommended value at 25 °C: 0.000 37 Pa		Wania <i>et al.</i> 1994
3,3',4,4'-tetrachloro-(PCB-77)	25	0.002 29, 0.001 96	GC-RT, supercooled liq., value	Bidleman 1984
	25	0.00213, 0.00144, 0.000207	GC-RT, supercooled liq., value	Foreman & Bidleman 1985
		$\log p/\text{Pa} = 12.62 - 4532/T$	GC-RT, supercooled liq.	Falconer & Bidleman 1994
		recommended value at 25 °C: 0.000 06 Pa		
2,2',4,5,5'-pentachloro-(PCB-101)	25	9.60 × 10 ⁻⁴	gas saturation-GC	Westcott & Bidleman 1981
	25	0.0016	GC-retention time	
	25	9.60×10^{-4}	gas saturation	Westcott <i>et al.</i> 1981
	30	1.73×10^{-3}		
	30–40	$\log p/\text{Torr} = 11.10 - 4840/T$	gas saturation, Antoine eq.	Westcott <i>et al.</i> 1981
	30–40	0.0012	GC-retention data	Bidleman <i>et al.</i> 1983
	25	0.00173	gas saturation-GC	
	30	0.000 96	GC-RT data	
	30–40	$\log p/\text{mmHg} = 11.28 - 4870/T$	gas saturation data	Bidleman 1984
	25	0.005 03, 0.003 16	GC-RT, supercooled liq., value	Foreman & Bidleman 1985
	25	0.0361, 0.004 03, 0.003 67	GC-RT, supercooled liq., value	
	5–45	$\log p/\text{mmHg} = 11.0 - 4750/T$	GC-retention data	Tateya <i>et al.</i> 1988
	25	0.003 15, 0.002 96	GC-RT, supercooled liq.	Hinckley <i>et al.</i> 1990
		$\log p/\text{Pa} = 12.13 - 4369/T$	GC-RT, supercooled liq.	
		$\log p/\text{Pa} = 12.67 - 4514/T$	GC-RT, supercooled liq.	Falconer & Bidleman 1994
		recommended value at 25 °C: 0.001 Pa		
2,2',3,3',4,4'-hexachloro-(PCB-128)	25	$(3.412, 92, 3, 41) \times 10^{-4}$	GC-RT, supercooled liq., values	Foreman & Bidleman 1985
	5–45	$\log p/\text{mmHg} = 11.40 - 5020/T$	GC-RT, supercooled liq.	Tateya <i>et al.</i> 1988
		$\log p/\text{Pa} = 12.91 - 4881/T$	GC-RT, supercooled liq.	Falconer & Bidleman 1994
		recommended value at 25 °C:		

TABLE 3. Vapor pressures and reported equations of chlorobenzenes, chlorinated dioxins and dibenzofurans, t in °C and T in K—Continued

Compounds	$t^{\circ}\text{C}$ or temp range	p/Pa	Method	Reference
2,2',4,4',5,5'-hexachloro- (PCB-153)	25 25 5–45	0.000 68, 0.000 72 0.000 708, 0.000 813, 0.00 070 $\log p/\text{mmHg} = 11.40 - 5040/T$ $\log p/\text{Pa} = 12.85 - 4775/T$	GC-RT, supercooled liq. value GC-RT, supercooled liq. value GC-RT, supercooled liquid GC-RT, supercooled liquid	Bidleman 1984 Foreman & Bidleman 1985 Tateya <i>et al.</i> 1988 Falconer & Bidleman 1994
2,2',4,4',6,6'-hexa- (PCB-155)	25 25 –10 0 10 20 30	recommended value at 25 °C 0.001 73 $\log p/\text{mmHg} = 11.05 - 4750/T$ $\log p/\text{Pa} = 12.02 - 4303/T$ 1.634×10^{-6} 1.185×10^{-5} 8.039×10^{-5} 3.250×10^{-4} 7.780×10^{-4}	GC-RT, supercooled liq. value GC-RT data, supercooled liq.- extrapolated GC-RT GC-RT data, supercooled liq. gas saturation	Bidleman <i>et al.</i> 1983 Burkhard <i>et al.</i> 1985 Falconer & Bidleman 1994 Wania <i>et al.</i> 1994
2,2',3,3',4,4',5-hepta- (PCB-170)	25 25	recommended value at 25 °C: $(5.0 \pm 0.5) \times 10^{-4}$ Pa 8.37×10^{-5} $(8.73, 8.11, 8.13) \times 10^{-5}$	GC-RT, supercooled liq. value GC-RT, supercooled liq. value GC-RT, supercooled liq.	Bidleman 1984 Foreman & Bidleman 1985 Falconer & Bidleman 1994
2,2',3,3',5,5',6,6'-octa- (PCB-202)	29–61.2 25 29 39.9 50 61.2 25 25 25 25	recommended value at 25 °C: $\log p/\text{Pa} = 13.282, 5307.3/T$ 2.90×10^{-5} 4.95×10^{-5} 2.24×10^{-4} 5.83×10^{-4} 2.65×10^{-3} 2.89×10^{-6} 3.91×10^{-4} $6.59 \times 10^{-4}, 5.2610^{-4}$ $\log p/\text{Pa} = 12.99 - 4851/T$ $\log p/\text{Pa} = 12.99 - 4851/T$	gas saturation, Antoine eq. gas saturation-GC	Wania <i>et al.</i> 1994 Burkhard <i>et al.</i> 1984
decachlorobiphenyl (PCB-209)	25 50.7 64.9 72.3 80.5 85.2 89.8	recommended value at 25 °C: $(3.5 \pm 0.5) \times 10^{-5}$ Pa 5.30×10^{-8} 2.69×10^{-6} 1.68×10^{-5} 4.00×10^{-5} 1.43×10^{-4} 1.88×10^{-4} 3.36×10^{-4}	extrapolated expd data, solid GC-RT, supercooled liq. value GC-RT, supercooled liq. GC-RT, supercooled liq.	Burkhard <i>et al.</i> 1985 Foreman & Bidleman 1985 Hinckley <i>et al.</i> 1990 Hinckley <i>et al.</i> 1990 Falconer & Bidleman 1994
decachlorobiphenyl (PCB-209)	25 25 25	$\log p/\text{Pa} = 14.049 - 6358.0/T$ 5.30×10^{-8} 1.32×10^{-5} $5.14 \times 10^{-6}, 1.44 \times 10^{-5}$	gas saturation-GC data, Antoine eq. extrapolated expd data, solid GC-RT, supercooled liq. value GC-RT, supercooled liq. values GC-RT, supercooled liq. GC-RT, supercooled liq.	Burkhard <i>et al.</i> 1984 Burkhard <i>et al.</i> 1985 Foreman & Bidleman 1985 Hinckley <i>et al.</i> 1990 Falconer & Bidleman 1994 Goodman 1997
decachlorobiphenyl (PCB-209)	25	$\log p/\text{Pa} = 13.27 - 5402/T$ 2.60×10^{-5}	Knudsen effusion method	

TABLE 3. Vapor pressures and reported equations of chlorobenzenes, chlorinated dioxins and dibenzofurans, t in °C and T in K—Continued

Compounds	t /°C or temp range	p /Pa	Method	Reference
PCB-209 (cont'd)	70	5.10×10^{-5}		
	75	8.10×10^{-5}		
	80	1.10×10^{-4}		
	85	1.80×10^{-4}		
	85–85	$\log p/\text{Pa} = 9.91 - 4886/T$	Knudsen effusion, Antoine eq.	Goodman 1997
		recommended value at 25 °C: $(5.0 \pm 0.5) \times 10^{-5}$ Pa		
Dioxins:				
dibenzo- <i>p</i> -dioxin	25	0.055	25–125 °C	gas saturation
	50	0.98		Rordorf 1985, 1986, 1989
	75	12		Rordorf 1989
	100	97		
	125	630		
	25	0.055		
		recommended value at 25 °C: 0.55 Pa		
	25	0.012	25–125 °C	gas saturation
	50	0.26		
	75	3.6		
	100	36		
	125	260		
		recommended value at 25 °C: 0.012 Pa		
	25	0.017	25–125 °C	gas saturation
	50	0.36		Rordorf 1987, 1989
	75	4.8		
	100	45		
	125	320		
		recommended value at 25 °C: 0.017 Pa		
	25	0.00039	25–125 °C	gas saturation-GC,
	50	0.0011		Rordorf 1987, 1989
	75	0.18		
	100	2.20		
	125	19		
		recommended value at 25 °C: 0.0004 Pa		
	25	0.00012	25–125 °C	gas saturation-GC,
	50	0.0033		Rordorf 1987, 1989
	75	0.056		
	100	0.64		
	125	5.40		
		recommended value at 25 °C: 0.00012 Pa		
	25	0.00014	25–125 °C	gas saturation-GC,
	50	0.0042		Rordorf 1987, 1989
	75	0.078		
	100	0.97		
	125	8.80		
		recommended value at 25 °C: 0.00014 Pa		
	25	0.0001	25–125 °C	gas saturation-GC,
	50	0.0042		Rordorf 1987, 1989
1,2,4-TCDD				

TABLE 3. Vapor pressures and reported equations of chlorobenzenes, chlorinated dioxins, and dibenzofurans, t in °C and T in K—Continued

Compounds	$t/^\circ\text{C}$ or temp range	P/Pa	Method	Reference
1,2,4-TCDD (cont'd)	75	0.10		
	100	1.60		
	125	18		
	recommended value at 25 °C: 0.0001 Pa			
1,2,3,4-TCDD	25	1.44×10^{-4}	GC-RT, supercooled liq. value	Eitzer & Hites 1988, 1991
	25	6.40×10^{-6}	gas saturation	Rordorf 1987, 1989
	50	2.60×10^{-4}		
	75	0.0062		
	100	0.092		
	125	1.10		
	25	6.37×10^{-4}	GC-RT, corrected p_L	Eitzer & Hites 1998
	recommended value at 25 °C: 6.4×10^{-6} Pa			
1,3,6,8-TCDD	20	5.37×10^{-4}		
	50	1.32×10^{-3}	gas saturation,	Webster <i>et al.</i> 1985
	100	1.12×10^{-3}		
	25	7.00×10^{-7}		
	50	3.60×10^{-5}		
	75	1.00×10^{-3}		
	100	1.90×10^{-2}		
	125	0.240		
	recommended value at 25 °C: 7.0×10^{-7} Pa			
2,3,7,8-TCDD	30.1	4.65×10^{-7}		
	30.2	5.19×10^{-7}	gas saturation-GC/MS,	Schroy <i>et al.</i> 1985a
	30.3	8.73×10^{-7}		
	54.6	2.06×10^{-5}		
	55.	1.37×10^{-5}		
	55.2	1.94×10^{-5}		
	61.9	3.71×10^{-5}		
	62	4.58×10^{-5}		
	70.9	1.79×10^{-4}		
	71	1.58×10^{-4}		
	71.1	1.59×10^{-4}		
	25	2.02×10^{-7}		
		$\ln p/Pa = 34.570834 - 14.903438/T$	gas saturation, Antoine eq.	Schroy <i>et al.</i> 1985a
	30.1	4.67×10^{-7}		Schroy <i>et al.</i> 1985b
	54.6	1.83×10^{-5}		
	62	4.97×10^{-5}		
	71	1.59×10^{-4}		
	10-305	$\log P/\text{mmHg} = 12.89784 + [6477.132/(273.15+t)]$	Antoine eq.	
	305-420	$\log P/\text{mmHg} = 12.89784 + [6477.132/(273.15+t)]$	Antoine eq.	
	20	8.71×10^{-6}	gas saturation-LSC	Webster <i>et al.</i> 1985
	50	1.12×10^{-5}		
	100	1.72×10^{-5}	gas saturation-LSC	Podoll <i>et al.</i> 1986
	25	9.87×10^{-8}	gas saturation-GC	Rordorf 1985, 1987, 1989
	25	2.00×10^{-7}		
	50	9.50×10^{-6}		

TABLE 3. Vapor pressures and reported equations of chlorobenzenes, chlorinated dioxins and dibenzofurans, t in °C and T in K—Continued

Compounds	t /°C or temp range	P /Pa	Method	Reference
2,3,7,8-TCDD (cont'd)	75	2.60×10^{-4}		
	100	4.60×10^{-3}		
	125	5.70×10^{-2}		
	25	2.53×10^{-7}	GC-RT correlation, solid	Eitzer & Hites 1988, 1991
1,2,3,4,7-PCDD	recommended value at 25 °C: 2.0×10^{-7} Pa	8.80×10^{-8}	predicted, solid	Rordorf 1987, 1989
	25	6.40×10^{-6}		
	50	2.50×10^{-4}		
	75	6.10×10^{-3}		
	100	9.80×10^{-2}		
	125			
1,2,3,7,8-PCDD	recommended value at 25 °C: 8.8×10^{-8} Pa	5.80×10^{-8}	predicted, solid	Rordorf 1987, 1989
	25	3.80×10^{-6}		
	50	1.40×10^{-4}		
	75	3.00×10^{-3}		
	100	4.60×10^{-2}		
	125	1.75×10^{-5}	GC-RT correlation, supercooled liq.	Eitzer & Hites 1988, 1991
1,2,3,4,7,8-H ₆ CDD	recommended value at 25 °C: 5.8×10^{-8} Pa	1.25×10^{-4}	GC-RT correlation, corrected p_L	Eitzer & Hites 1998
	25	5.10×10^{-9}	predicted, solid	Rordorf 1987, 1989
	50	4.10×10^{-7}		
	75	1.80×10^{-5}		
	100	4.60×10^{-4}		
	125	8.00×10^{-3}		
	25	8.09×10^{-4}	GC-RT, supercooled liq. value	Eitzer & Hites 1988, 1991
	25	3.18×10^{-5}	GC-RT, corrected p_L	Eitzer & Hites 1998
1,2,3,4,6,7,8-H ₇ CDD	recommended value at 25 °C: 5.1×10^{-9} Pa	7.50×10^{-10}	predicted	Rordorf 1987, 1989
	25	8.00×10^{-8}		
	50	4.40×10^{-6}		
	75	1.40×10^{-4}		
	100	2.90×10^{-3}		
	125	1.024×10^{-6}	GC-RT, supercooled liq. value	Eitzer & Hites 1988, 1991
Octachloro-	recommended value at 25 °C: 7.5×10^{-10} Pa	8.97×10^{-6}	GC-RT, corrected p_L	Eitzer & Hites 1998
	25	2.77×10^{-7}	GC-RT, supercooled liq. value	Eitzer & Hites 1988, 1991
	25	1.10×10^{-10}	gas saturation-GC,	Rordorf 1987, 1989
Dibenzofurans:				
dibenzofuran	30	0.4874	GC-RT, corrected p_L	Eitzer & Hites 1998
	35	0.7818	30–70 °C	Hansen & Eckert 1986

TABLE 3. Vapor pressures and reported equations of chlorobenzenes, chlorinated dioxins and dibenzofurans, t in °C and T in K—Continued

Compounds	t /°C or temp range	p /Pa	Method	Reference
DBF (cont'd)				
	40	1.28		
	45	2.128		
	50	3.20		
	55	4.679		
	60	7.246		
	65	12.78		
	70	19.71		
	25	0.2762		
	30–70	$\log p/mPa = 16.30 - 4132/T$	Antoine eq.-exptl. data	Hansen & Eckert 1986
	130–286	$\log p_L/kPa = 5.8968 - 1851.27/(T - 82.64)$	Antoine eq., liquid	Stephenson & Malnowski 1987
	25	0.35	gas saturation-GC,	Rordorf 1987, 1989
	50	5.1		
	75	50		
	100	360		
	125	2100		
2,8-dichlorodibenzofuran	25	recommended value at 25 °C: 0.35 Pa	25–125 °C	
	50	3.90×10^{-4}	gas saturation-GC,	
	75	9.10×10^{-3}		
	100	0.140		
	125	1.40		
		11.0		
2,4,8-trichlorodibenzofuran	25	recommended value at 25 °C: 3.9×10^{-4} Pa	25–125 °C	
	50	9.10×10^{-5}	gas saturation-GC,	
	75	3.00×10^{-3}		
	100	0.0610		
	125	0.820		
		8.00		
2,3,7,8-TCDF	25	recommended value at 25 °C: 9.1×10^{-5} Pa	25–125 °C	
	25	1.23×10^{-4}	GC-RT, supercooled liq. value	Eitzer & Hites 1988, 1991
	25	2.00×10^{-6}	predicted,	Rordorf 1989
	50	8.50×10^{-5}		
	75	2.10×10^{-3}		
	100	0.0330		
	125	0.380		
	25	7.506×10^{-4}	GC-RT, corrected p_L	Eitzer & Hites 1998
1,2,3,7,8-PCDF	25	recommended value at 25 °C:		
	25	3.64×10^{-5}	$25-125^{\circ}\text{C}$	
	25	2.30×10^{-7}	GC-RT, supercooled liq. value	Eitzer & Hites 1988, 1991
	50	1.30×10^{-5}	predicted,	Rordorf 1989
	75	4.00×10^{-4}		
	100	8.00×10^{-3}		
	125	0.110		
	25	2.30×10^{-7}	GC-RT, corrected p_L	Eitzer & Hites 1998
2,3,4,7,8-PCDF	25	recommended value at 25 °C: 2.3×10^{-7} Pa	$25-125^{\circ}\text{C}$, solid	Eitzer & Hites 1988, 1991
	25	2.17×10^{-5}	GC-RT, supercooled liq. value	Rordorf 1989
		3.50×10^{-7}	predicted,	

TABLE 3. Vapor pressures and reported equations of chlorobenzenes, chlorinated dioxins and dibenzofurans, t in °C and T in K—Continued

Compounds	t /°C or temp range	p /Pa	Method	Reference
2,3,4,7,8-PCDF (cont'd)	50	2.10×10^{-5}		
	75	6.70×10^{-4}		
	100	0.0140		
	125	0.190		
1,2,3,4,6,7,8-heptachloro-	25 recommended value at 25 °C: 3.5×10^{-5} Pa	3.88×10^{-5}	GC-RT, corrected p_L	Eitzer & Hites 1998
	25	2.24×10^{-6}		
	25	4.70×10^{-9}		
	50	4.30×10^{-7}		
	75	2.00×10^{-5}		
	100	5.80×10^{-4}		
	125	1.10×10^{-2}		
	25 recommended value at 25 °C:	1.84×10^{-5}	GC-RT correlation, corrected p_L	Eitzer & Hites 1998
1,2,3,4,7,8,9-heptachloro-	25	1.31×10^{-6}		
	25	6.20×10^{-9}		
	50	7.20×10^{-7}		
	75	3.60×10^{-5}		
	100	1.00×10^{-3}		
	125	2.00×10^{-2}		
octachlorodibenzofuran	25 recommended value at 25 °C:	5.0×10^{-10}	gas saturation-GC,	Rordorf 1986, 1989
	50	5.30×10^{-8}		
	75	2.90×10^{-6}		
	100	9.10×10^{-5}		
	125	1.90×10^{-3}		
	25 recommended value at 25 °C: 5.08×10^{-10} Pa	5.0×10^{-10}		

Note:
 GC - gas chromatography
 RT - retention time
 LSC - liquid scintillation counting
 DD - dibenzo-*p*-dioxin

DCDD - dichlorodibenz-*p*-dioxin
 TCDD - tri- or tetrachlorodibenz-*p*-dioxin
 PCDD - pentachlorodibenz-*p*-dioxin
 H_6 CDD - hexachlorodibenz-*p*-dioxin
 H_7 CDD - heptachlorodibenz-*p*-dioxin
 OCDD - octachlorodibenz-*p*-dioxin
 DF - dibenzofuran
 TCDF - tri- or tetrachlorodibenzofuran
 PCDF - pentachlorodibenzofuran
 p_L -liquid or supercooled liquid vapor pressure

TABLE 4. Henry's law constants and reported equations of chlorobenzenes, chlorinated dioxins and dibenzofurans

Compound	t/°C or temp range	Henry's law constant H/(Pa·m³/mol)	Method	Ref.
chlorobenzene	25	383	gas stripping	Mackay <i>et al.</i> 1979
	25	314	gas stripping	Mackay & Shiu 1981
	21	124	equilibration cell,	Leighton & Calo 1981
	3	125	(concentration ratio-GC)	
	12.4	190		
	12.5	206		
	17.9	243		
	19.1	280		
	22.7	271		
	23	321		
	1–23	ln K/atm = 18.46 – 3751/T		
	25	398	gas stripping	Warner <i>et al.</i> 1987
	20	319	EPICS	Yurteri <i>et al.</i> 1987
	10	247	EPICS	Ashworth <i>et al.</i> 1988
	15	285		
	20	346		
	25	365		
	30	479		
	10–30	H/(atm·m³/mol) = exp(3.469 – 2689/T)		
	45	621	equilibrium headspace-GC	Ettre <i>et al.</i> 1993
	60	863		
	70	1114		
	80	1579		
	45–80	log(1/K _{AW}) = –2.905 024 0 + 1129.8083/T		
	25	367	gas stripping	Shiu & Mackay 1997
		K _{AW} = 0.122 · 10 ⁷ [– 1507(1/T – 1/293)]		Staudinger & Roberts 1996
	20	288	inert gas stripping	Hovorka & Dohnal 1997
	21	293	headspace equilibrium	de Wolf & Lieder 1998
		recommended value at 25 °C: 368 Pa·m³/mol		
1,2-dichlorobenzene	25	193	gas stripping	Mackay & Shiu 1981
	20	121.6	gas stripping	Oliver 1985
	25	197	gas stripping	Warner <i>et al.</i> 1987
	10	165	EPICS	Ashworth <i>et al.</i> 1988
	15	145		
	20	170		
	25	159		
	30	240		
	10–30	H/(atm·m³/mol) = exp(–1.518 – 1422/T)		
	25	244.2	gas stripping	Ashworth <i>et al.</i> 1988
		K _{AW} = 0.0547 · 10 ⁷ [– 2436(1/T – 1/293)]		Shiu & Mackay 1997
	20	141	gas stripping	Staudinger & Roberts 1996
		recommended value at 25 °C: 178 Pa·m³/mol		Hovorka & Dohnal 1997
1,3-dichlorobenzene	20	186	gas stripping	Oliver 1985
	25	266	gas stripping	Warner <i>et al.</i> 1987
	10	224	EPICS	Ashworth <i>et al.</i> 1988
	15	234		
	20	298		
	25	289		
	30	428		
	10–30	H/(atm·m³/mol) = exp(2.882 – 2564/T)		
	20	216	gas stripping	Ashworth <i>et al.</i> 1988
	21	269	headspace equil.	Horvoka & Dohnal 1997
		recommended value at 25 °C: 318.5 Pa·m³/mol		de Wolf & Lieder 1998
1,4-dichlorobenzene	25	240	gas stripping	Mackay & Shiu 1981
	20	152	gas stripping	Oliver 1985
	25	276	gas stripping	Warner <i>et al.</i> 1987
	20	190	EPICS	Yurteri <i>et al.</i> 1987
	10	215	EPICS	Ashworth <i>et al.</i> 1988
	15	220		
	20	262		
	25	321		
	30	394		
	10–30	H/(atm·m³/mol) = exp(3.373 – 2720/T)		Ashworth <i>et al.</i> 1988

TABLE 4. Henry's law constants and reported equations of chlorobenzenes, chlorinated dioxins and dibenzofurans—Continued

Compound	<i>t</i> /°C or temp range	Henry's law constant <i>H</i> /(Pa·m ³ /mol)	Method	Ref.
1,4-DCB (cont'd)	25	244	gas stripping	Shiu & Mackay 1997
	20	188	gas stripping	Horvoka & Dohnal 1997
	20	663	direct conc ratio	Chiang <i>et al.</i> 1998
	20	936	EPICS gas-phase	
	20	395	EPICS liquid-phase	
	recommended value at 25 °C: 239 Pa·m ³ /mol			
1,2,3-trichlorobenzene	25	127		Mackay & Shiu 1981
	20	90.2	gas stripping	Oliver 1985
	20	72	gas stripping	ten Hulscher <i>et al.</i> 1992
	25	127		Shiu & Mackay 1997
	recommended value at 25 °C: 130 Pa·m ³ /mol			
1,2,4-trichlorobenzene	20	121.6	gas stripping	Oliver 1985
	25	144	gas stripping	Warner <i>et al.</i> 1987
	10	131	EPICS	Ashworth <i>et al.</i> 1988
	15	106		
	20	185		
	25	195		
	30	301		
	10–30	$H/(atm\cdot m^3/mol) = \exp(7.261 - 4028/T)$		Ashworth <i>et al.</i> 1988
	recommended value at 25 °C: 181 Pa·m ³ /mol			
1,3,5-trichlorobenzene	20	193	gas stripping	Oliver 1985
	20	192	gas stripping	ten Hulscher <i>et al.</i> 1992
	recommended value at 25 °C: 567 Pa·m ³ /mol			
1,2,3,4-tetrachlorobenzene	20	69.9	gas stripping	Oliver 1985
	14.8	38.5	gas stripping	ten Hulscher <i>et al.</i> 1992
	20	62		
	20.1	52		
	22.1	68.1		
	24.1	70.9		
	34.8	129.9		
	50.5	276.2		
	$\ln H/(Pa\cdot m^3/mol) = 21.1804 - 5027.9/T$			
	recommended value at 25 °C: 144 Pa·m ³ /mol			
1,2,3,5-tetrachlorobenzene	25	159	gas stripping	Mackay & Shiu 1981
	20	99	gas stripping	ten Hulscher <i>et al.</i> 1992
	25	160	gas stripping	Shiu & Mackay 1997
	recommended value at 25 °C: 306 Pa·m ³ /mol			
1,2,4,5-tetrachlorobenzene	20	101	gas stripping	Oliver 1985
	recommended value at 25 °C: 239 Pa·m ³ /mol			
pentachlorobenzene	20	71.94	gas stripping	Oliver 1985
	14.8	37.4	gas stripping	ten Hulscher <i>et al.</i> 1992
	20	59		
	20.1	49.4		
	22.1	68.1		
	24.1	66.7		
	34.8	124.1		
	50.5	276.2		
	$\ln H/(Pa\cdot m^3/mol) = 21.4142 - 5108/T$; regression			
	recommended value at 25 °C: 110 Pa·m ³ /mol			
hexachlorobenzene	23	134	gas stripping	Atlas <i>et al.</i> 1982
	23	71.4	gas stripping-LSC	Atlas <i>et al.</i> 1983
	20	48.4	gas stripping	Oliver 1985
	25	172	batch stripping	Warner <i>et al.</i> 1987
	14.8	23.6	batch stripping	ten Hulscher <i>et al.</i> 1992
	20	41		
	20.1	30		
	22.1	46.6		
	24.1	52.5		
	34.8	88.3		
	50.5	217.2		
	$\ln H/(Pa\cdot m^3/mol) = 22.7994 - 5630.6/T$			
	26	26243	EPICS	ten Hulscher <i>et al.</i> 1992
	46	29587		Hansen <i>et al.</i> 1993
	recommended value at 25 °C: 131 Pa·m ³ /mol			

TABLE 4. Henry's law constants and reported equations of chlorobenzenes, chlorinated dioxins and dibenzofurans—Continued

Compound	<i>t</i> /°C or temp range	Henry's law constant <i>H</i> /(Pa·m ³ /mol)	Method	Ref.
PCBs:				
2-chlorobiphenyl	25	74.6		Dow Chemical Co. 1982
3-chlorobiphenyl	25	62.1		Dow Chemical Co. 1982
4-chlorobiphenyl	25	58.06		Dow Chemical Co. 1982
2,2'-dichloro-	23	22.3	equil. concn ratio	Murphy <i>et al.</i> 1983
	20	30.19	equil. concn ratio	Murphy <i>et al.</i> 1987
	25	34.17	gas stripping	Dunnivant & Elzerman 1988
	25	34.17	gas stripping	Dunnivant <i>et al.</i> 1988
	25	24.79	wetted-wall column	Fendinger & Glotfelty 1990
	25	23.3	wetted-wall column	Brunner <i>et al.</i> 1990
	recommended value at 25 °C			
2,4'-dichloro-	23	96.03	gas stripping	Atlas <i>et al.</i> 1982
	23	22.29	equil. concn ratio	Murphy <i>et al.</i> 1983
	20	23.31	equil. concn ratio	Murphy <i>et al.</i> 1987
2,5-dichlorobiphenyl	25	39.31	gas stripping	Dunnivant & Elzerman 1988
	14.8	16.1	gas stripping	ten Hulscher <i>et al.</i> 1992
	20	29.6		
	30.1	58.2		
	34.9	82.2		
	42.1	123		
	47.9	163.4		
	$\ln H/(Pa \cdot m^3/mol) = 24.9242 - 6339.7/T$			ten Hulscher <i>et al.</i> 1992
	recommended value at 25 °C:			ten Hulscher <i>et al.</i> 1992
3,3'-dichloro-	25	23.61	gas stripping	Dunnivant & Elzerman 1988
3,4-dichloro-	25	20.77	gas stripping	Dunnivant & Elzerman 1988
4,4'-dichloro-	25	20.16	gas stripping	Dunnivant & Elzerman 1988
	25	9.67	wetted-wall column	Fendinger & Glotfelty 1990
2,2',3-trichloro-	23	101	gas stripping	Atlas <i>et al.</i> 1982
	23	81.8	equil. concn ratio	Murphy <i>et al.</i> 1983
	25	20.27	wetted-wall column	Brunner <i>et al.</i> 1990
2,2',5-trichloro-	23	81.25	gas stripping	Atlas <i>et al.</i> 1982
	23	35.00	equilibrium	Murphy <i>et al.</i> 1983
	20	20.27	gas stripping	Oliver 1985
	20	24.11	equil. concn ratio	Murphy <i>et al.</i> 1987
	25	25.33	wetted-wall column	Brunner <i>et al.</i> 1990
2,3,3'-trichloro-	23	81.25	gas stripping	Atlas <i>et al.</i> 1982
	25	20.27	wetted-wall column	Brunner <i>et al.</i> 1990
2,3',5-trichloro-	20	34.35	equil. concn ratio	Murphy <i>et al.</i> 1987
	25	32.93	gas stripping	Dunnivant & Elzerman 1988
	25	32.93	gas stripping	Dunnivant <i>et al.</i> 1988
	25	20.27	wetted-wall column	Brunner <i>et al.</i> 1990
2,3,6-trichloro-	20	32.12	equil. concn ratio	Murphy <i>et al.</i> 1987
	25	22.29	wetted-wall column	Brunner <i>et al.</i> 1990
2,4,4'-trichloro-	20	26.75	equil. concn ratio	Murphy <i>et al.</i> 1987
	25	20.25	wetted-wall column	Brunner <i>et al.</i> 1990
	10.4	8.7	gas stripping	ten Hulscher <i>et al.</i> 1992
	20	21.2		
	30.1	47.4		
	34.9	50.3		
	42.1	70.8		
	47.9	120.6		
	48.4	122.2	gas stripping	ten Hulscher <i>et al.</i> 1992
	$\ln H/(Pa \cdot m^3/mol) = 23.616 - 6052/T$			
	recommended value at 25 °C:			
2,4,5-trichloro-	25	20.27	wetted-wall column	Brunner <i>et al.</i> 1990
2,4',5-trichloro-	23	93.56	gas stripping	Atlas <i>et al.</i> 1982

TABLE 4. Henry's law constants and reported equations of chlorobenzenes, chlorinated dioxins and dibenzofurans—Continued

Compound	<i>t</i> /°C or temp range	Henry's law constant <i>H</i> /(Pa·m ³ /mol)	Method	Ref.
2,4',5-TC (cont'd)	23	20.26	equil. concn ratio	Murphy <i>et al.</i> 1983
	20	26.75	equil. concn ratio	Murphy <i>et al.</i> 1987
	25	19.25	wetted-wall column	Brunner <i>et al.</i> 1990
2,4,6-trichloro-	25	65.76	gas stripping	Dunnivant & Elzerman 1988
	23	83.71	gas stripping	Atlas <i>et al.</i> 1982
3,4,4'-trichloro-	20	15.4	equil. concn ratio	Murphy <i>et al.</i> 1987
	25	10.18	wetted-wall column	Brunner <i>et al.</i> 1990
	20	12.16	gas stripping	Oliver 1985
2,2,3,3'-tetrachloro-	20	16.31	gas stripping	Murphy <i>et al.</i> 1987
	25	20.47	gas stripping	Dunnivant & Elzerman 1988
	25	20.47	gas stripping	Dunnivant <i>et al.</i> 1988
2,2',3,5'-tetrachloro-	25	20.27	wetted-wall column	Brunner <i>et al.</i> 1990
	23	78.79	gas stripping	Atlas <i>et al.</i> 1982
2,2',4,6'-tetrachloro-	23	24.32	equil. concn ratio	Murphy <i>et al.</i> 1983
	20	19.15	equil. concn ratio	Murphy <i>et al.</i> 1987
	23	76.33	gas stripping	Atlas <i>et al.</i> 1982
2,2',5,5'-tetrachloro-	23	93.56	gas stripping	Atlas <i>et al.</i> 1982
	rm temp	22.3	equilibrium	Murphy <i>et al.</i> 1983
2,2,5,6'-tetrachloro-	20	12.16	gas stripping	Oliver 1985
	25	2.53	gas stripping	Hassett & Milicic 1985
	20	24.12	equil. concn ratio	Murphy <i>et al.</i> 1987
	25	40.88	gas stripping	Dunnivant & Elzerman 1988
	25	40.88	gas stripping	Dunnivant <i>et al.</i> 1988
2,2',6,6'-tetrachloro-	25	20.27	wetted-wall column	Brunner <i>et al.</i> 1990
	10.4	8.6	gas stripping	ten Hulscher <i>et al.</i> 1992
2,3,4,4'-tetrachloro- 3,3',4,4'-tetrachloro-	20	16.4		
	30.1	37.4		
	34.9	38.8		
	42.1	68.7		
	47.9	109.2		
	48.4	120.6		
	$\ln H/(Pa \cdot m^3/mol) = 23.9459 - 6192.6/T$ recommended value at 25 °C: 47.7 Pa·m ³ /mol			
	25	41.14	gas stripping	Dunnivant & Elzerman 1988
	25	20.27	wetted-wall column	Brunner <i>et al.</i> 1990
	25	55.73	gas stripping	Dunnivant & Elzerman 1988
2,3,4,4'-tetrachloro- 3,3',4,4'-tetrachloro-	23	20.27	wetted-wall column	Brunner <i>et al.</i> 1990
	23	83.17	gas stripping	Atlas <i>et al.</i> 1982
	25	9.52	gas stripping	Dunnivant & Elzerman 1988
2,2',4,5,5'-pentachloro-	23	27	equilibrium	Murphy <i>et al.</i> 1983
	20	7.09	gas stripping	Oliver 1985
	20	18.14	equil. concn ratio	Murphy <i>et al.</i> 1987
	25	25.43	gas stripping	Dunnivant & Elzerman 1988
	25	25.43	gas stripping	Dunnivant <i>et al.</i> 1988
2,2',3,3',4,4'-hexachloro-	25	9.12	wetted-wall column	Brunner <i>et al.</i> 1990
	20	5.78	equil. concn ratio	Murphy <i>et al.</i> 1987
	25	3.06	gas stripping	Dunnivant & Elzerman 1988
2,2',4,4',5,5'-hexachloro-	20	1.32	wetted-wall column	Brunner <i>et al.</i> 1990
	20	6.08	gas stripping	Oliver 1985
	20	10.03	equil. concn ratio	Murphy <i>et al.</i> 1987
	25	13.37	gas stripping	Dunnivant & Elzerman 1988
2,2',4,4',6,6'-hexachloro-	25	13.4, 12.5	gas stripping	Dunnivant <i>et al.</i> 1988
	25	2.73	wetted-wall column	Brunner <i>et al.</i> 1990
	25	76.5	gas stripping	Dunnivant & Elzerman 1988

TABLE 4. Henry's law constants and reported equations of chlorobenzenes, chlorinated dioxins and dibenzofurans—Continued

Compound	t/°C or temp range	Henry's law constant <i>H</i> /(Pa·m ³ /mol)	Method	Ref.
2,2,3,3'5,5'6,6'-octa-Dioxins: dibenzo- <i>p</i> -dioxin	25	76.5, 11.65 18.24	gas stripping wetted-wall column	Dunnivant <i>et al.</i> 1988 Brunner <i>et al.</i> 1990
2,7-DCDD	25	5.96	equil of concurrent column	Santl <i>et al.</i> 1994
1,2,4-TCDD	25	3.64	equil of concurrent column	Santl <i>et al.</i> 1994
1,2,3,4-TeCDD	25	2.02	equil of concurrent column	Santl <i>et al.</i> 1994
Dibenzofurans: 2,3,7,8-TCDF	25	1.7	gas stripping	Friesen <i>et al.</i> 1993

Note:

H - Henry's law constant in units of Pa·m³/mol or atm·m³/mol,

K - Henry's law constant in unit of pressure, atm,

*K*_{AW} - air-water partition coefficient or dimensionless Henry's law constant,

EPICS - Equilibrium Partitioning In Closed System.

TABLE 5. Summary of physical-chemical properties recommended at 25 °C and equations for 5–50 °C, temperature t in °C and T in K

Compound	Recommended properties at 25 °C		Recommended temperature dependence equations between 5 and 50 °C	Calcd value at 25 °C
chlorobenzene	p , Pa	1580±30	$\log p/kPa=6.115\ 12-1438.86/(T-54.72)$	1600 Pa
	S , g/m ³	484±20	$\ln x=-41.9062+6054.03/T+1.3692\times 10^{-4}\cdot T^2$	501.5 g/m ³
	H , Pa·m ³ /mol	368		
1,2-DCB	p , Pa	170±20	$\log p/kPa=19.40-6013/T$	171 Pa
	S , g/m ³	140±20	$\ln x=-31.5289+3834/T+8.7172\times 10^{-5}\cdot T^2$	148 g/m ³
	H , Pa·m ³ /mol	178		
1,3-DCB	p , Pa	260±30	$\ln p/\text{Pa}=21.6433-4031.27/(T-47.5846)$	258.6 Pa
	S , g/m ³	120±20	N/A	
	H , Pa·m ³ /mol	318.5		
1,4-DCB	p , Pa	130±20	$\log p/\text{Pa}=11.632\ 09-2829.32/T$	138.8 Pa
	S , g/m ³	80±10	$\ln x=-4.178-2186.7/T$	81.7 g/m ³
	H , Pa·m ³ /mol	239		
1,2,3-TCB	p , Pa	15±5	$\log p/kPa=9.787-3440/T$	17.7 Pa
	S , g/m ³	21±4	$\ln x=-1.773-3418.9/T$	14.5 g/m ³
	H , Pa·m ³ /mol	130		
1,2,4-TCB	p , Pa	40±4	$\log p/kPa=9.570-3254/T$; solid: 6–17 °C	38.70 Pa
	S , g/m ³	40±4	$\log p/kPa=6.682-2064.4/(T-43.05)$; liquid 20–110 °C	
	H , Pa·m ³ /mol	181	N/A	
1,3,5-TCB	p , Pa	25±3.0	$\log p/kPa=8.301-2956/T$	24.3 Pa
	S , g/m ³	8.0±1.0	$\ln x=-5.083\ 768-2650.68/T$	8.60 g/m ³
	H , Pa·m ³ /mol	567		
1,2,3,4-TeCB	p , Pa	5.2±1.0	N/A	
	S , g/m ³	7.0±3	N/A	
	H , Pa·m ³ /mol	144		
1,2,3,5-TeCB	p , Pa	5.1±1.0	N/A	
	S , g/m ³	3.6±0.5	$\ln x=-4.4222-3162.74/T$	3.56 g/m ³
	H , Pa·m ³ /mol	306		
1,2,4,5-TeCB	p , Pa	0.72	N/A	
	S , g/m ³	0.60±0.10	$\ln x=-4.529-3708.6/T$	0.513 g/m ³
	H , Pa·m ³ /mol	259		
Pentachloro-	p , Pa	0.22±0.10	$\log p/\text{Pa}=15.6174-4831.4/T$	0.259 Pa
	S , g/m ³	0.50±0.10	$\ln x=-3.614\ 82-4093.10/T$	0.41 g/m ³
	H , Pa·m ³ /mol	110		
HCB	p , Pa	0.0023±0.0005	$\log p/\text{Pa}=10.83-4044/T$	0.001 85 Pa
	S , g/m ³	0.005±0.001	$\ln x=-8.229\ 56-4037.26/T$	0.005 53 g/m ³
	H , Pa·m ³ /mol	131		
PCBs:				
PCB-1	p , Pa	1.0±0.2	$\log p/kPa=9.99-3893/T$	0.86 Pa
	S , g/m ³	5.5±0.5	NR	
	H , Pa·m ³ /mol	34.3		
PCB-2	p , Pa	1.0±0.3	$\log p/\text{Pa}=11.641\ 78-3514.98/T$	0.712 Pa
	S , g/m ³	2.5	NR	
	H , Pa·m ³ /mol	75.5		
PCB-3	p , Pa	0.20±0.10	$\log p/\text{Pa}=15.188-4751.1/T$	0.180 Pa
	S , g/m ³	1.50±0.30	$\ln x=-5.9137-2926.22/T$	1.55 g/m ³
	H , Pa·m ³ /mol	25.2		
PCB-15	p , Pa	0.005±0.002	$\log p/\text{Pa}=14.10-4977/T$	0.002 55 Pa
	S , g/m ³	0.06±0.01	$\ln x=-2.8677-4839.46/T$	0.062 g/m ³
	H , Pa·m ³ /mol	18.6		
PCB-29	p , Pa	0.132	N/A	
	S , g/m ³	0.14±0.03	$\ln x=-3.061\ 75-4633.86/T$	0.119 g/m ³
	H , Pa·m ³ /mol	24.3		
PCB-30	p , Pa	0.038	N/A	
	S , g/m ³	0.20±0.02	$\ln x=-4.5969-4004.7/T$	0.212 g/m ³
	H , Pa·m ³ /mol	48.9		
PCB-52	p , Pa	0.0049	N/A	
	S , g/m ³	0.03±0.015	N/A	
	H , Pa·m ³ /mol	47.7		
PCB-61	p , Pa	0.000 37	$\log p/\text{Pa}=12.10-4632/T$	0.000 37 Pa
	S , g/m ³	0.0177	$\ln x=-3.967-4970.5/T$	0.0177 g/m ³
	H , Pa·m ³ /mol	61.04		
PCB-77	p , Pa	0.000 06	N/A	

TABLE 5. Summary of physical-chemical properties recommended at 25 °C and equations for 5–50 °C, temperature t in °C and T in K—Continued

Compound	Recommended properties at 25 °C		Recommended temperature dependence equations between 5 and 50 °C	Calcd value at 25 °C
PCB-77 (cont'd)	S , g/m ³	0.0008±0.0002	$\ln x = -3.58245 - 6074.34/T$	6.4×10^{-4} g/m ³
	H , Pa·m ³ /mol	21.9		
PCB-101	p , Pa	0.0011	N/A	
	S , g/m ³	0.01	$\ln x = -8.026 - 3826.44/T$	0.0158 g/m ³
PCB-128	H , Pa·m ³ /mol	35.9	N/A	
	p , Pa	0.00002	N/A	
PCB-136	S , g/m ³	0.0006	N/A	
	H , Pa·m ³ /mol	12	N/A	
PCB-153	p , Pa	0.00012	N/A	
	S , g/m ³	0.001±0.0002	$\ln x = -13.37313 - 2445.3/T$	0.0086 g/m ³
PCB-155	H , Pa·m ³ /mol	42.5		
	p , Pa	0.0005±0.00005	$\log p/\text{Pa} = 14.84 - 5399/T$	0.00054 Pa
PCB-202	S , g/m ³	0.002±0.001	$\ln x = -8.9206 - 4112.07/T$	0.00274 g/m ³
	H , Pa·m ³ /mol	90.2		
PCB-206	p , Pa	0.000027	$\log p/\text{Pa} = 13.282 + 5307.3/T$	3.03×10^{-5} Pa
	S , g/m ³	0.0003±38.7	$\ln x = -5.34 - 6100/T$	1.49×10^{-4} g/m ³
PCB-209	H , Pa·m ³ /mol			
	p , Pa	1.90×10^{-7}	$\ln x = -7.4275 - 6004.5/T$	2.75×10^{-5} g/m ³
Dioxins:	S , g/m ³	0.000025		
	H , Pa·m ³ /mol	3.53		
DD	p , Pa	5.02×10^{-8}	$\log p/\text{Pa} = 14.049 - 6358/T$	5.30×10^{-8} Pa
	S , g/m ³	1.0×10^{-6}	$\ln x = -4.632 - 8001/T$	6.0×10^{-7} g/m ³
H, Pa·m ³ /mol		25		
1-MCDD	p , Pa	0.055	$\log p/\text{Pa} = -4820.43/T + 14.91018$	0.0552 Pa
	S , g/m ³	0.865±0.08	$\ln x = 4.1680 - 6087.88/T$	0.895 g/m ³
2-MCDD	H , Pa·m ³ /mol	11.7		
	p , Pa	0.012	$\log p/\text{Pa} = -5150.40/T + 15.35327$	0.012 Pa
2,3-DCDD	S , g/m ³	0.417	$\ln x = -4912.75/T - 0.68385$	0.428 g/m ³
	H , Pa·m ³ /mol	7.28		
2,7-DCDD	p , Pa	0.017	$\log p/\text{Pa} = -5071.88/T + 15.2463$	0.017 Pa
	S , g/m ³	0.295	$\ln x = -6448/T + 4.093418$	0.295 g/m ³
2,8-DCDD	H , Pa·m ³ /mol	14.6		
	p , Pa	0.00039	N/A	
1,2,4-TCDD	S , g/m ³	0.0149	$\ln x = -6173.64/T - 0.07859$	0.0155 g/m ³
	H , Pa·m ³ /mol	6.62		
1,2,3,4-TCDD	p , Pa	0.00012	$\log p/\text{Pa} = -5523.34/T + 14.60827$	1.21×10^{-4} Pa
	S , g/m ³	0.00375	$\ln x = -5543.9/T - 3.48833$	0.00361 g/m ³
1,2,3,7-TCDD	H , Pa·m ³ /mol	8.1		
	p , Pa	0.00014	$\log p/\text{Pa} = -5699.96/T + 15.25386$	0.000137 Pa
1,2,3,7,8-TCDD	S , g/m ³	0.0167	$\ln x = -5379/T - 2.54177$	0.0162 g/m ³
	H , Pa·m ³ /mol	2.12		
1,2,4,7-PCDD	p , Pa	0.0001	$\log p/\text{Pa} = -6235.45/T + 16.9148$	1.0×10^{-4} Pa
	S , g/m ³	0.00841	$\ln x = -2.4909 - 5626.95/T$	0.00842 g/m ³
1,2,3,4,7-HCDD	H , Pa·m ³ /mol	3.42		
	p , Pa	6.40×10^{-6}	$\log p/\text{Pa} = -6199.79/T + 15.59851$	6.37×10^{-6} Pa
1,2,3,4,7,8-HCDD	S , g/m ³	0.00055±0.0003	$\ln x = -3984/T - 10.5076$	0.00077 g/m ³
	H , Pa·m ³ /mol	3.75		
2,3,7,8-TCDD	p , Pa	1.0×10^{-6}	N/A	
	S , g/m ³	0.00042	N/A	
1,2,3,4,7-PCDD	H , Pa·m ³ /mol	0.767		
	p , Pa	2.0×10^{-7}	$\log p/\text{Pa} = -6482.7/T + 15.0391$	2.0×10^{-7} Pa
1,2,3,4,7,8-HCDD	S , g/m ³	1.93×10^{-5}	N/A	
	H , Pa·m ³ /mol	3.34		
1,2,3,4,7,8-HCDD	p , Pa	8.80×10^{-8}	$\log p/\text{Pa} = -7179.05/T + 17.02207$	8.78×10^{-8} Pa
	S , g/m ³	1.18×10^{-4}	N/A	
1,2,3,4,7,8-HCDD	H , Pa·m ³ /mol	0.266		
	p , Pa	5.10×10^{-9}	$\log p/\text{Pa} = -7087.08/T + 15.65106$	7.60×10^{-9} Pa
1,2,3,4,7,8-HCDD	S , g/m ³	4.42×10^{-6}	N/A	
	H , Pa·m ³ /mol	0.45		

TABLE 5. Summary of physical-chemical properties recommended at 25 °C and equations for 5–50 °C, temperature t in °C and T in K—Continued

Compound	Recommended properties at 25 °C		Recommended temperature dependence equations between 5 and 50 °C	Calcd value at 25 °C
H7CDD	p , Pa	7.50×10^{-10}	$\log p/\text{Pa} = -7820.06/T + 17.103\ 57$	7.50×10^{-10} Pa
	S , g/m ³	2.40×10^{-6}	N/A	
	H , Pa·m ³ /mol	0.133		
OCDD	p , Pa	1.10×10^{-10}	$\log p/\text{Pa} = -7629.38/T + 15.818\ 86$	1.70×10^{-10} Pa
	S , g/m ³	7.40×10^{-8}	N/A	
	H , Pa·m ³ /mol	0.684		
Dibenzofurans:				
DF	p , Pa	0.30 ± 0.05	$\log p/\text{Pa} = 13.171\ 92 - 4083/T$	0.30 Pa
	S , g/m ³	4.75 ± 0.20	$\ln x = -1.6385 - 3842.2/T$	4.60 g/m^3
	H , Pa·m ³ /mol	10.6		
2,8-DCDF	p , Pa	0.000 39	$\log p/\text{Pa} = 14.306\ 69 - 5281.67/T$	0.000 39 Pa
	S , g/m ³	0.0145	$\ln x = -2.515 - 5398.4/T$	0.0146 g/m^3
	H , Pa·m ³ /mol	6.38		
OCDF	p , Pa	5.0×10^{-10}	$\log p/\text{Pa} = 16.889\ 37 - 7808.74/T$	5.0×10^{-10} Pa
	S , g/m ³	1.16×10^{-6}	$\ln x = -5.0496 - 7455.1/T$	$2.19 \times 10^{-6} \text{ g/m}^3$
	H , Pa·m ³ /mol	0.191		

Note:

 p - vapor pressure in Pa S - aqueous solubility in g/m³ x - mole fraction solubility H - Henry's law constant in Pa·m³/mol

CB - chlorobenzene

DCB - dichlorobenzene

TCB - trichlorobenzene

TeCB - tetrachlorobenzene

HCB - hexachlorobenzene

PCB - polychlorobiphenyl

DD - dibenzo-*p* - dioxinMCDD - monochlorodibenzo-*p* - dioxinDCDD - dichlorodibenzo - *p* - dioxinTCDD - tetrachlorodibenzo - *p* - dioxinPCDD - pentachlorodibenzo - *p* - dioxinH₆CDD - hexachlorodibenzo - *p* - dioxinH₇CDD - heptachlorodibenzo - *p* - dioxinOCDD - octachlorodibenzo - *p* - dioxin

DF - dibenzofuran

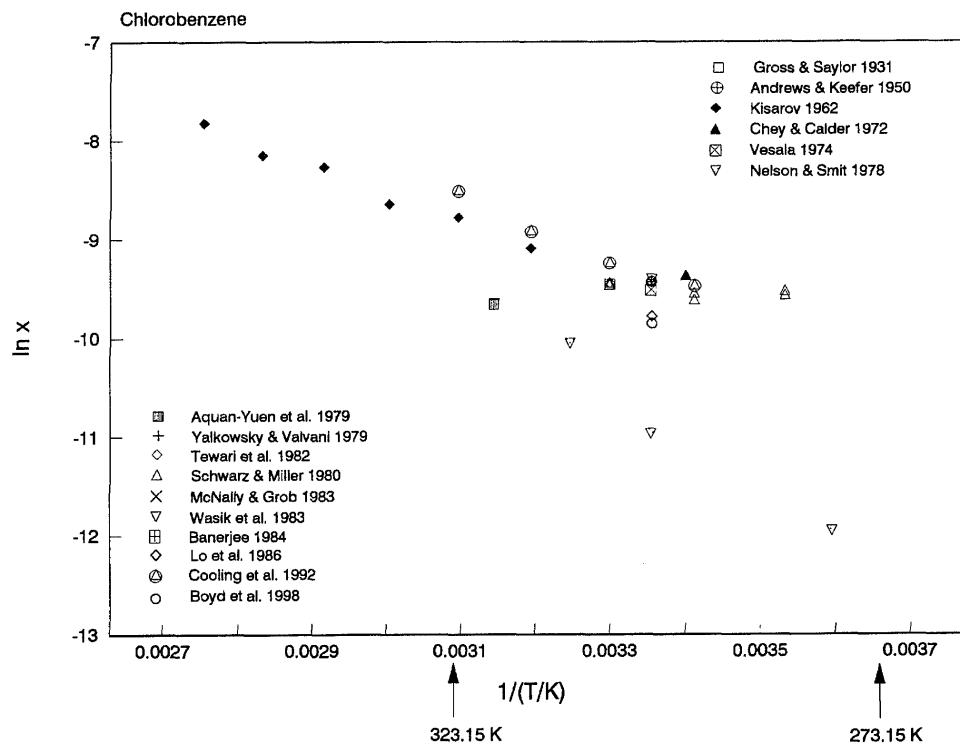
CDF - chlorodibenzofuran

DCDF - dichlorodibenzofuran

TCDF - tetrachlorodibenzofuran

OCDF - octachlorodibenzofuran

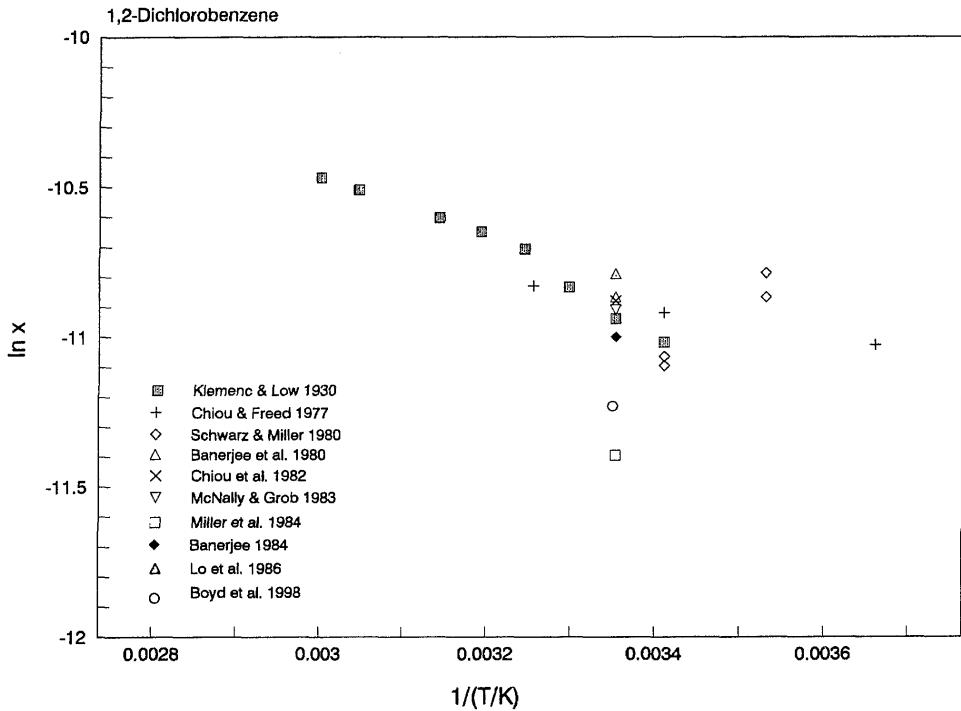
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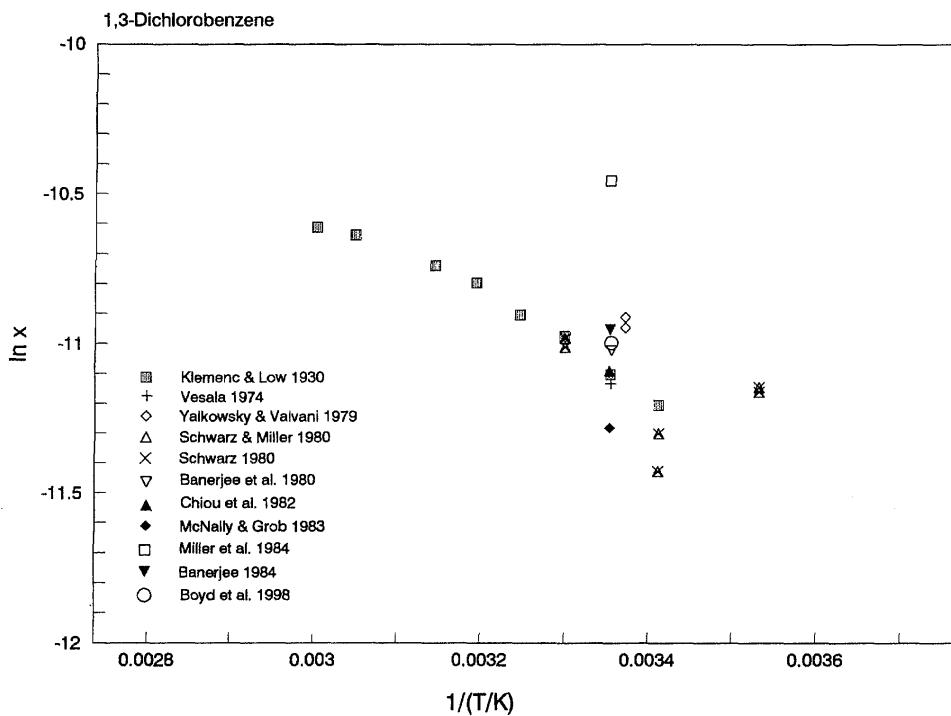
FIG. 1. Logarithm of mole fraction solubility vs $1/T$ for chlorobenzene.

from structure–property correlations are not reported. We believe that it is preferable that only measured data be used to predict and evaluate the environmental fate of organic chemicals. Because of the large quantity of reported vapor pressure data, the vapor pressure equation derived from re-

ported experimental data is selected and quoted as reported in the original publication. Correlation equations based on/or derived from experimental data from handbooks and/or review articles are also included.

Table 1 gives the physical constants of the chlorinated

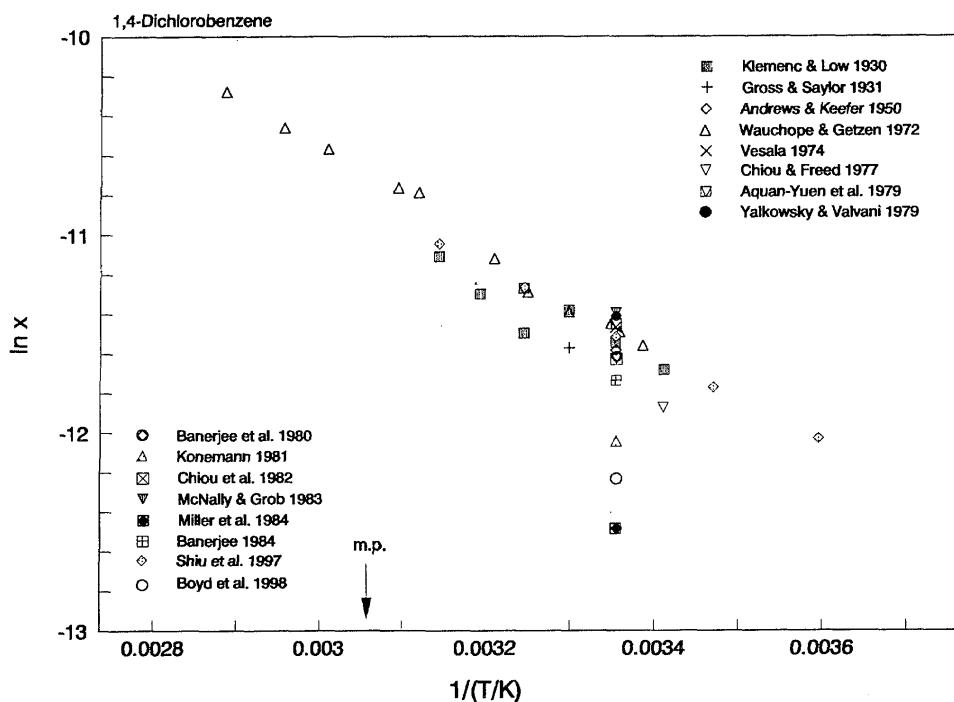
FIG. 2. Logarithm of mole fraction solubility vs $1/T$ for 1,2-dichlorobenzene.

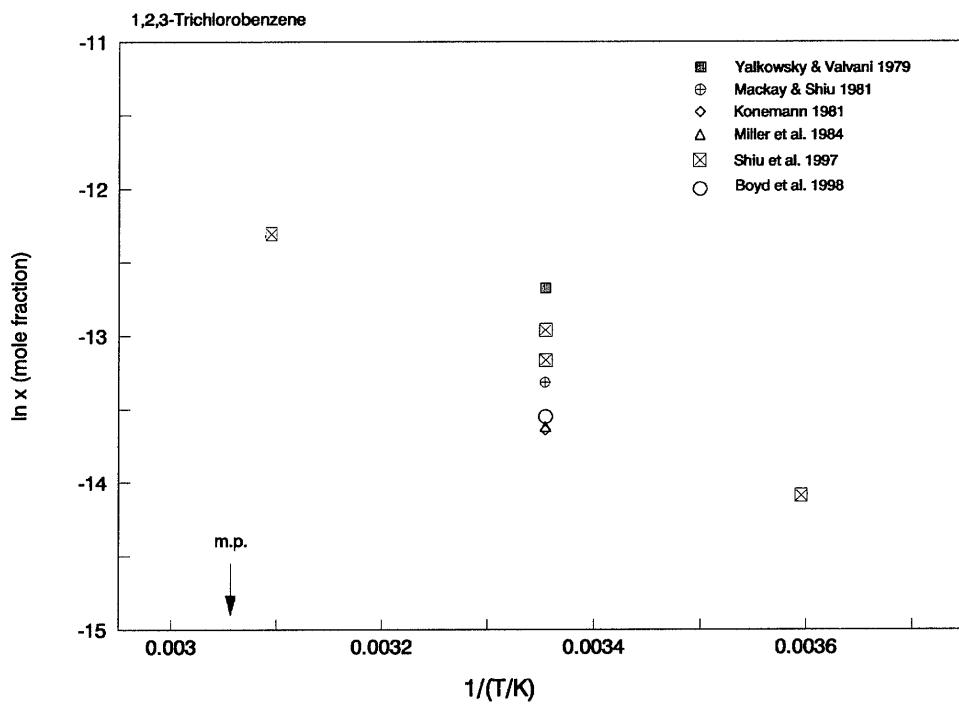
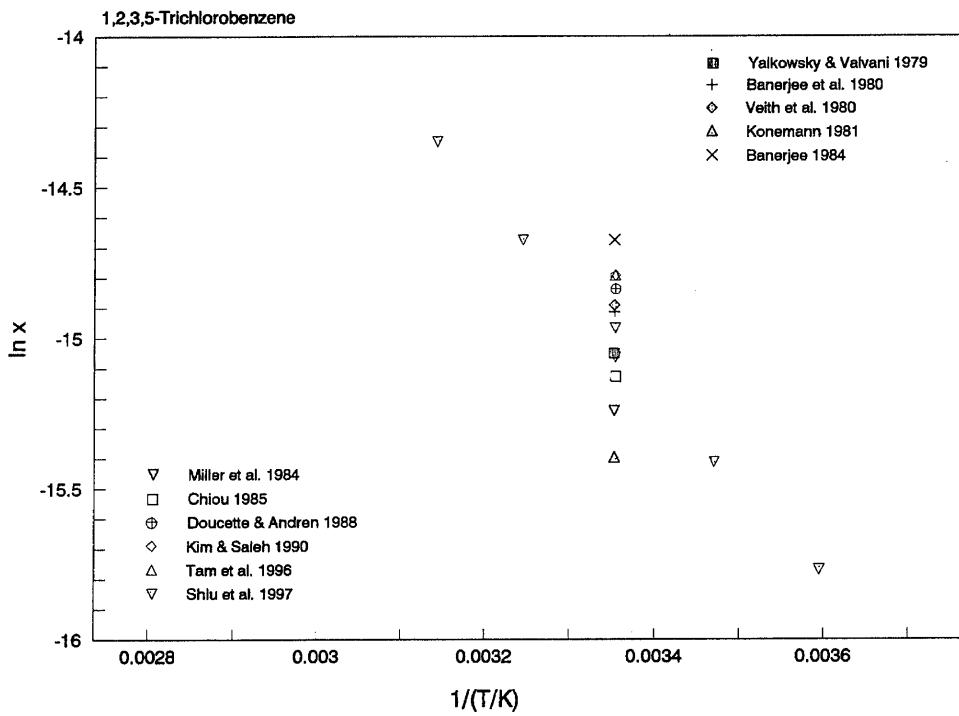
FIG. 3. Logarithm of mole fraction solubility vs $1/T$ for 1,3-dichlorobenzene.

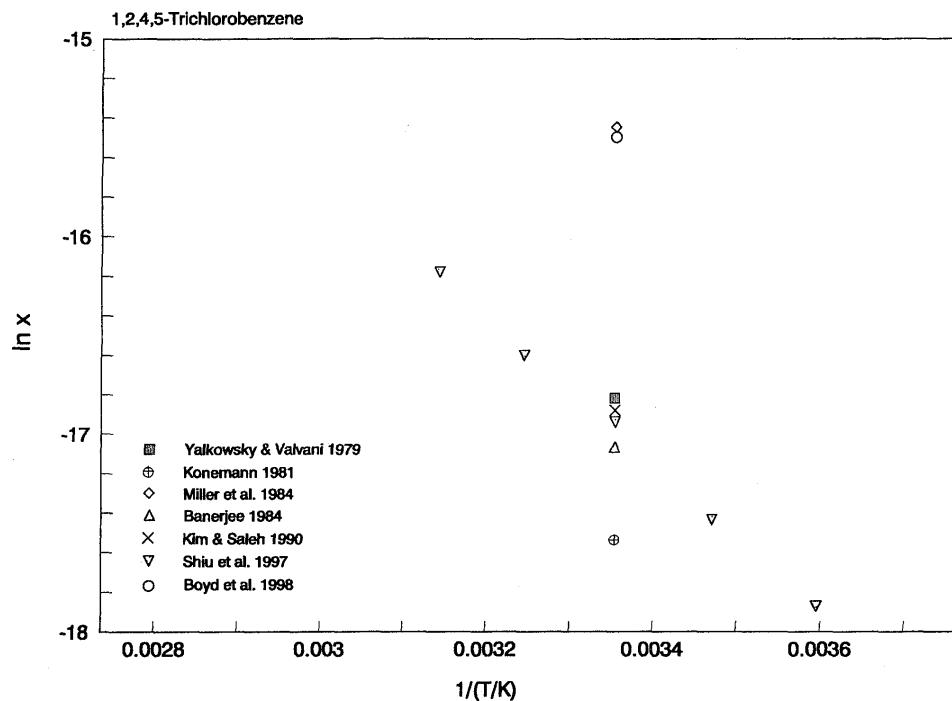
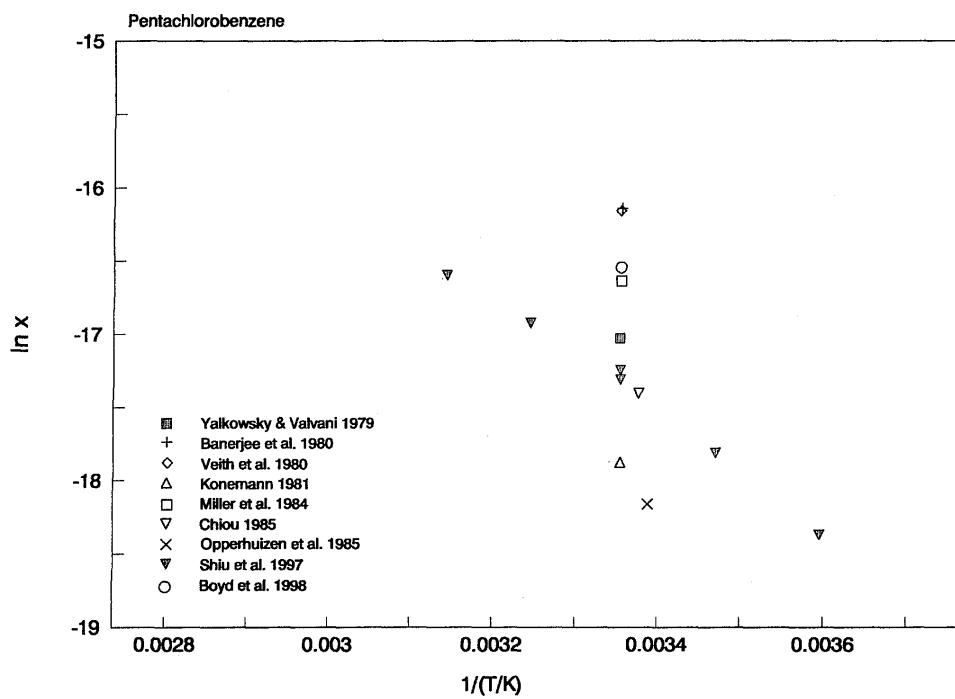
aromatic compounds, the enthalpies of fusion, enthalpies of vaporization, enthalpies of sublimation at reported temperatures, and references. Tables 2, 3 and 4 give the reported solubilities, vapor pressures, and Henry's law constants at reported temperatures, method of measurement and the reported equations expressed as function of temperatures.

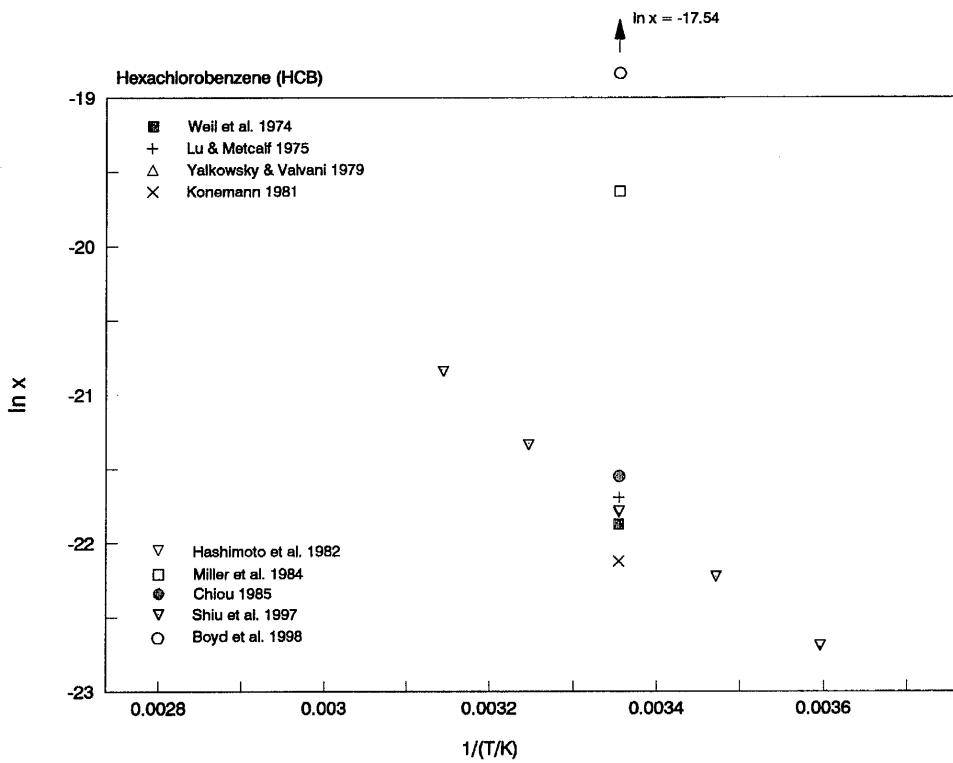
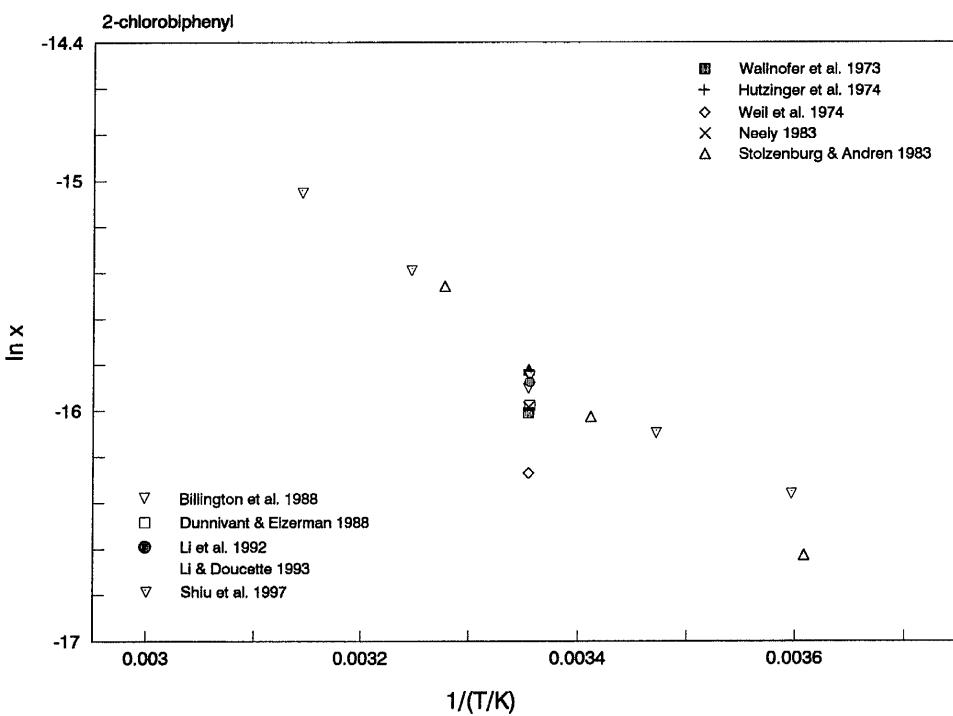
Table 5 gives the selected and recommended vapor pressures and solubilities at 25 °C and where possible, recommended temperature dependence equation between 5 and 50 °C are also given.

Plots of logarithm of aqueous solubility, vapor pressure and Henry's law constant are given in Figs. 1–48.

FIG. 4. Logarithm of mole fraction solubility vs $1/T$ for 1,4-dichlorobenzene.

FIG. 5. Logarithm of mole fraction solubility vs $1/T$ for 1,2,3-trichlorobenzene.FIG. 6. Logarithm of mole fraction solubility vs $1/T$ for 1,2,3,5-tetrachlorobenzene.

FIG. 7. Logarithm of mole fraction solubility vs $1/T$ for 1,2,4,5-tetrachlorobenzene.FIG. 8. Logarithm of mole fraction solubility vs $1/T$ for pentachlorobenzene.

FIG. 9. Logarithm of mole fraction solubility vs $1/T$ for hexachlorobenzene.FIG. 10. Logarithm of mole fraction solubility vs $1/T$ for 2-chlorobiphenyl.

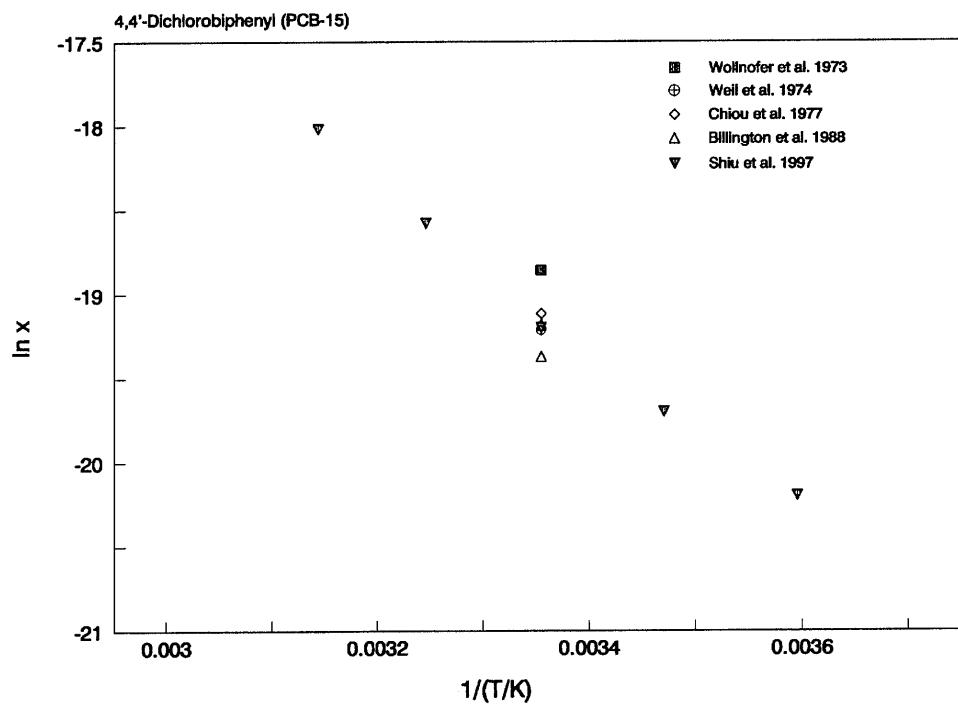


FIG. 11. Logarithm of mole fraction solubility vs $1/T$ for 4,4'-dichlorobiphenyl.

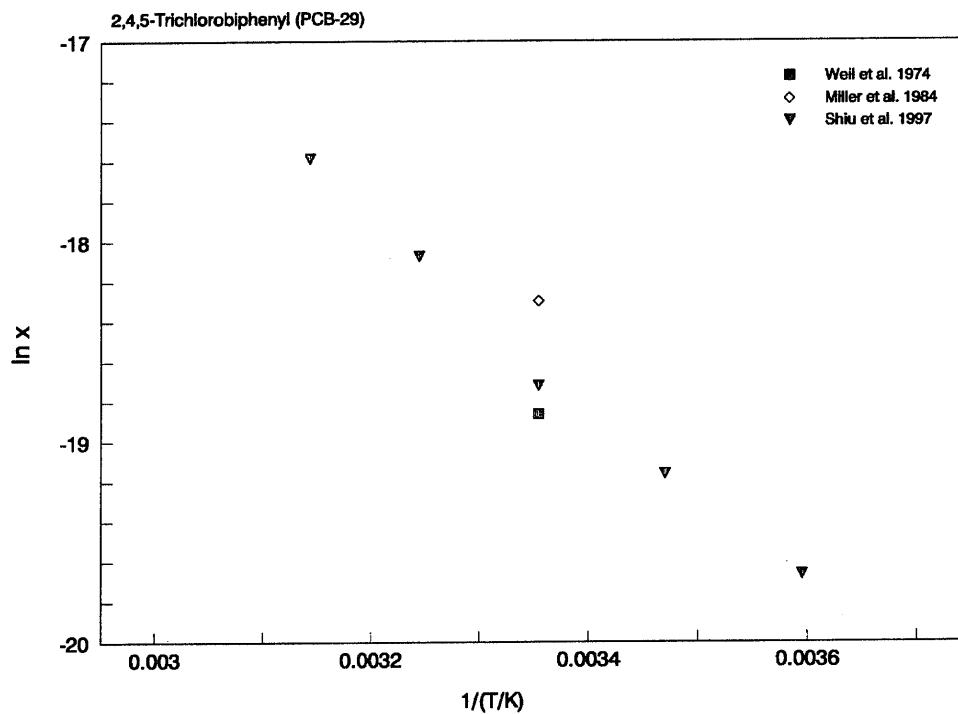
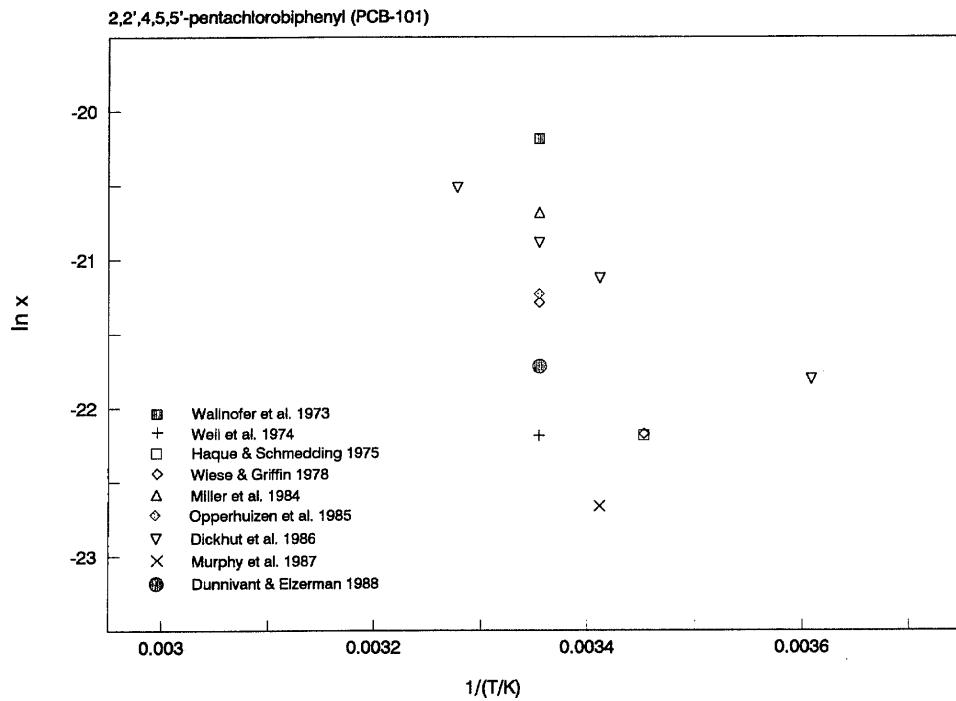
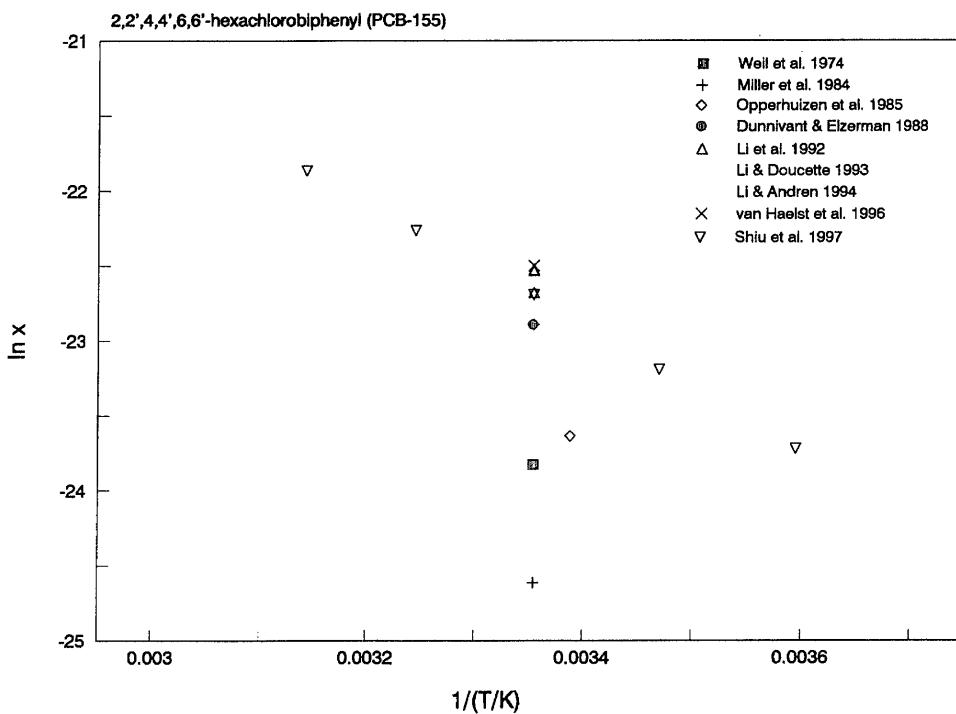
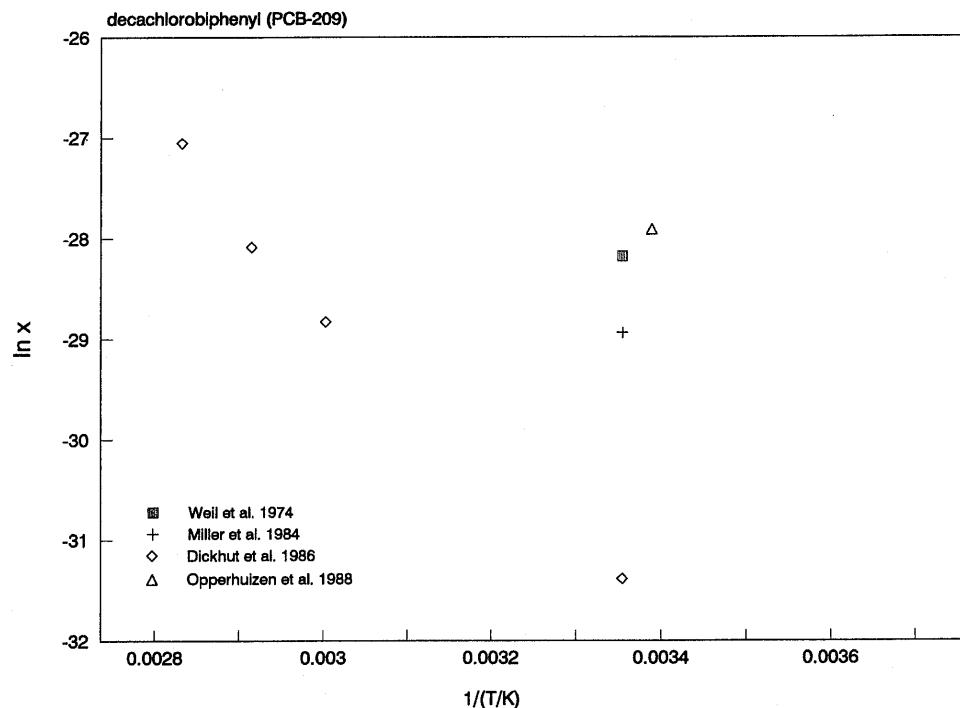
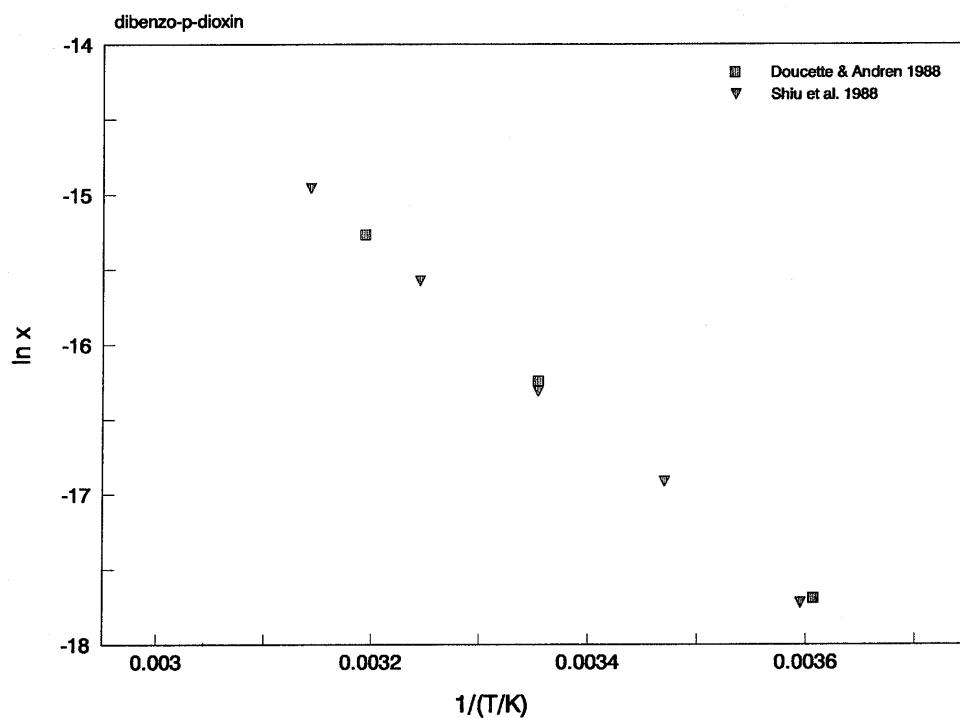
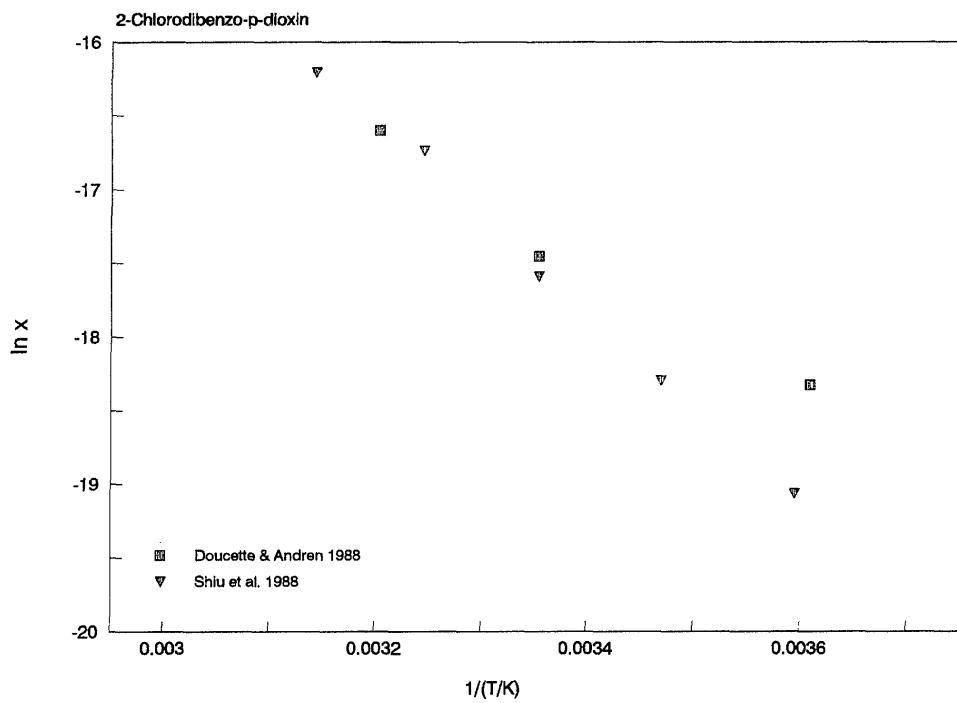
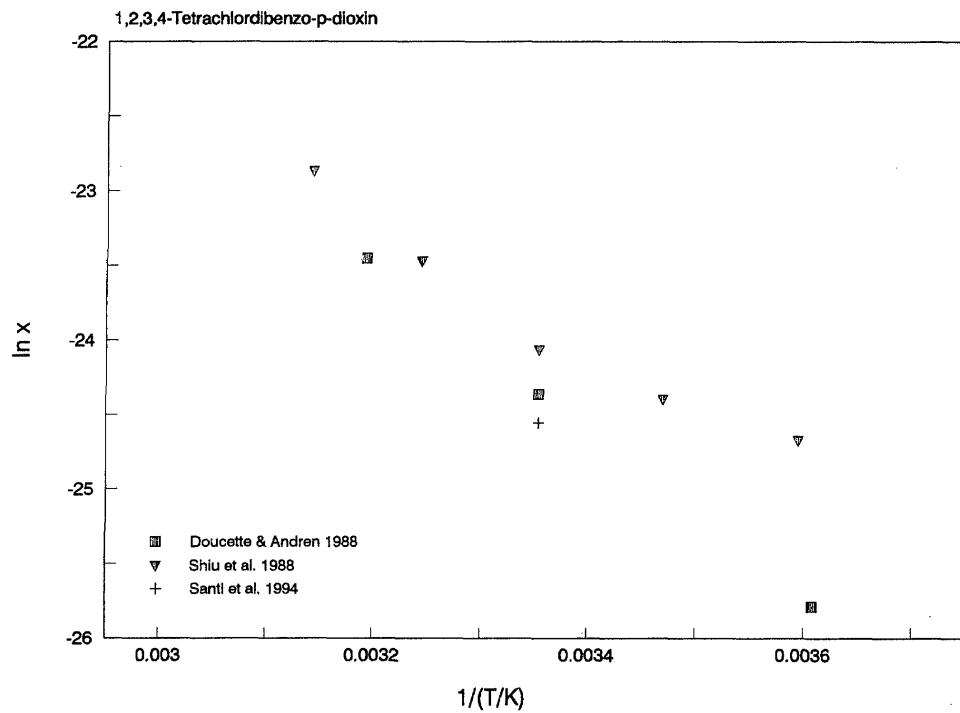
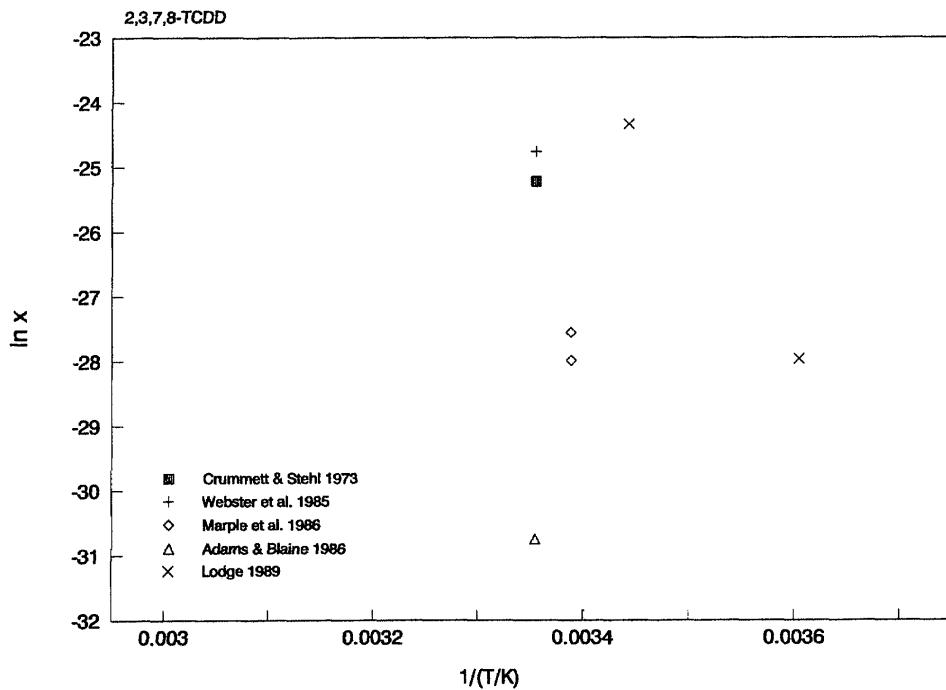
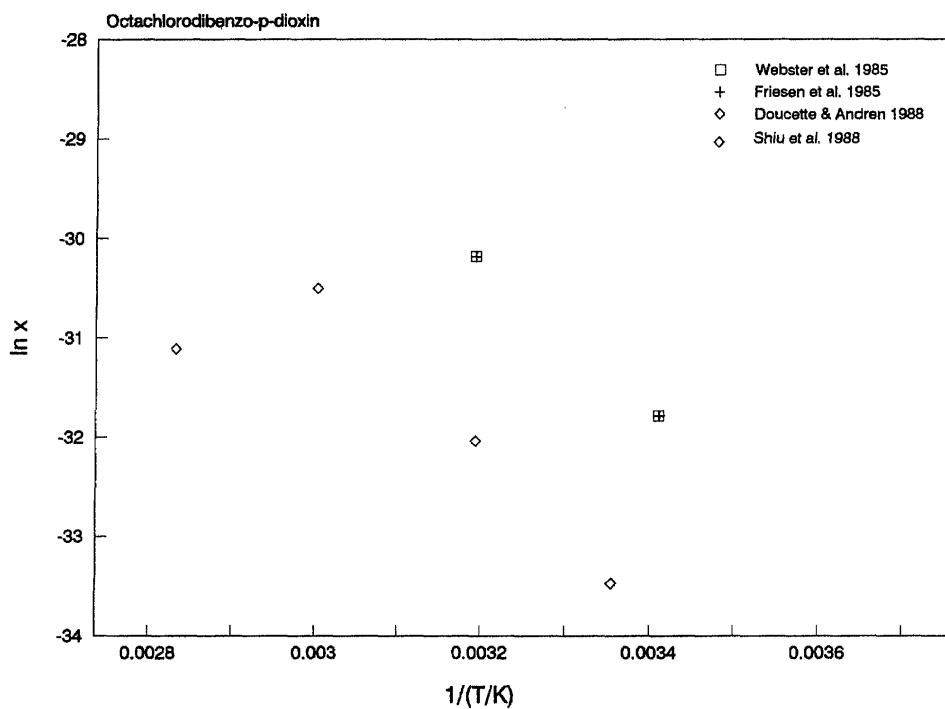


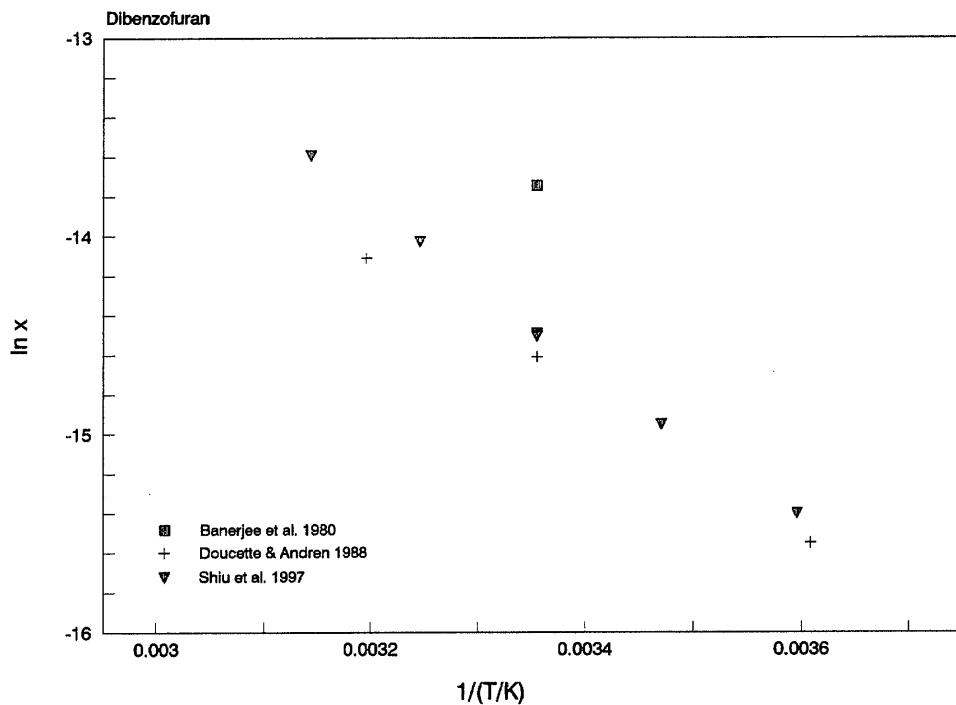
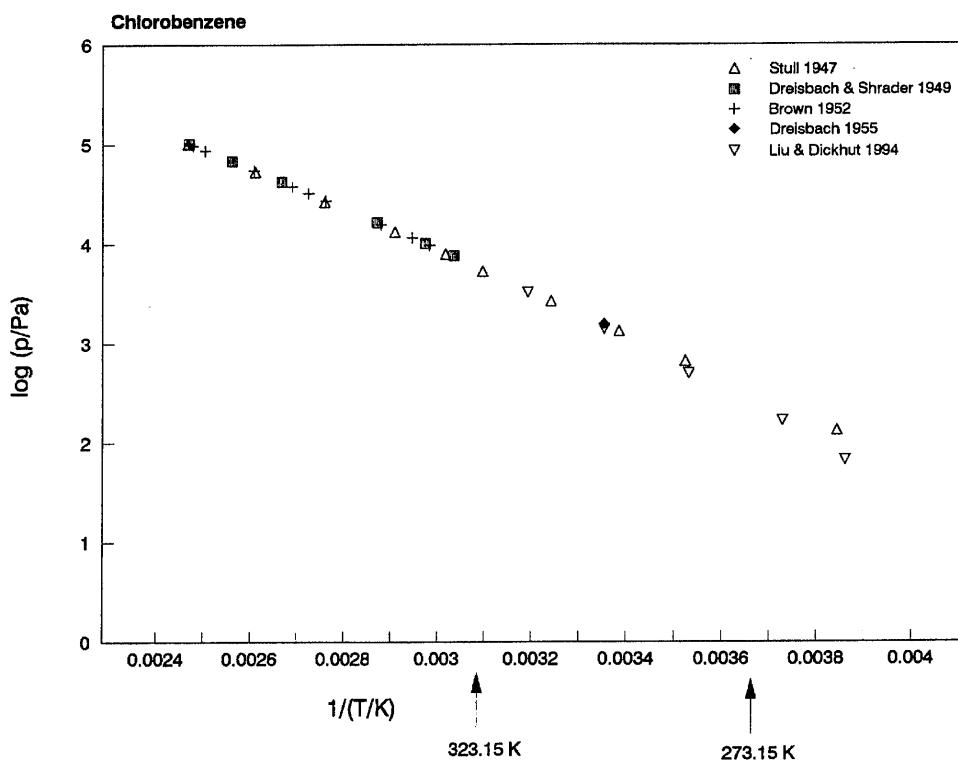
FIG. 12. Logarithm of mole fraction solubility vs $1/T$ for 2,4,5-trichlorobiphenyl.

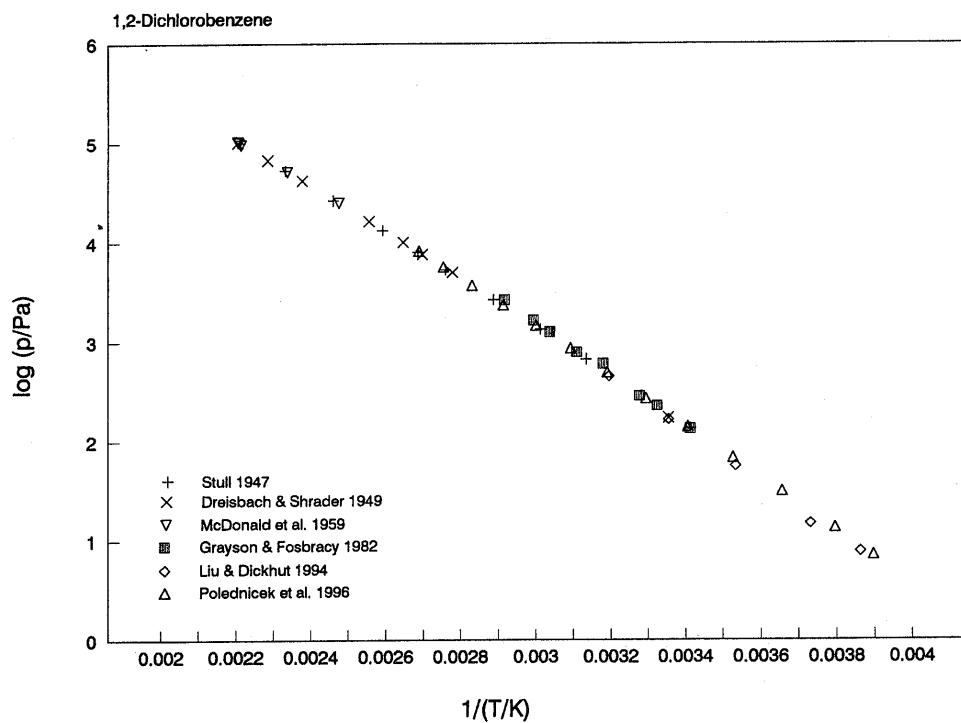
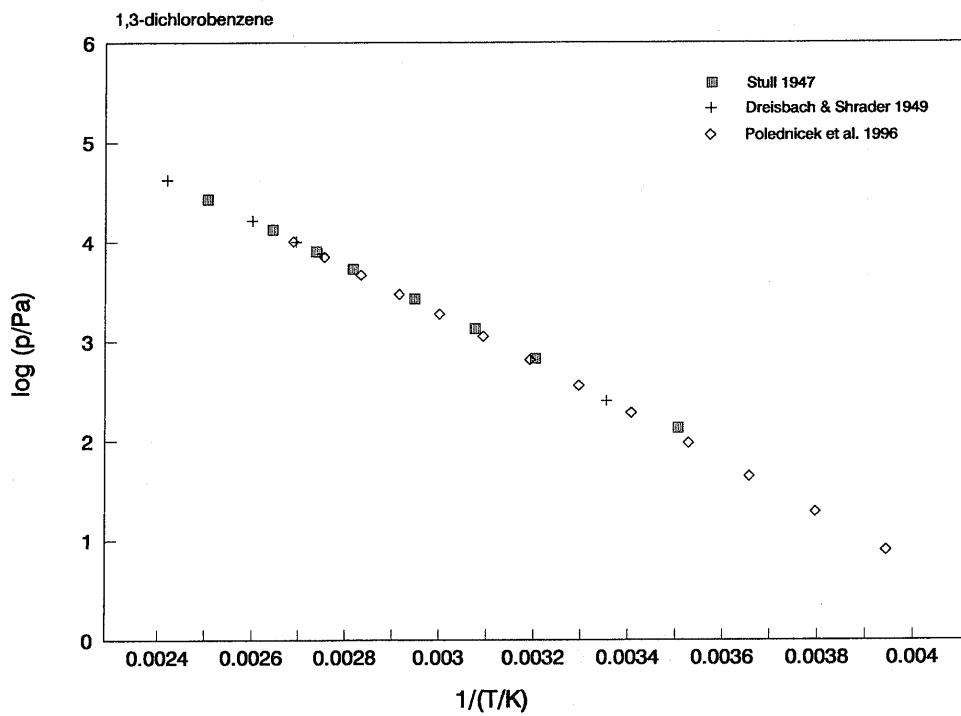
FIG. 13. Logarithm of mole fraction solubility vs $1/T$ for 2,2',4,5,5'-pentachlorobiphenyl.FIG. 14. Logarithm of mole fraction solubility vs $1/T$ for 2,2',4,4',6,6'-hexachlorobiphenyl.

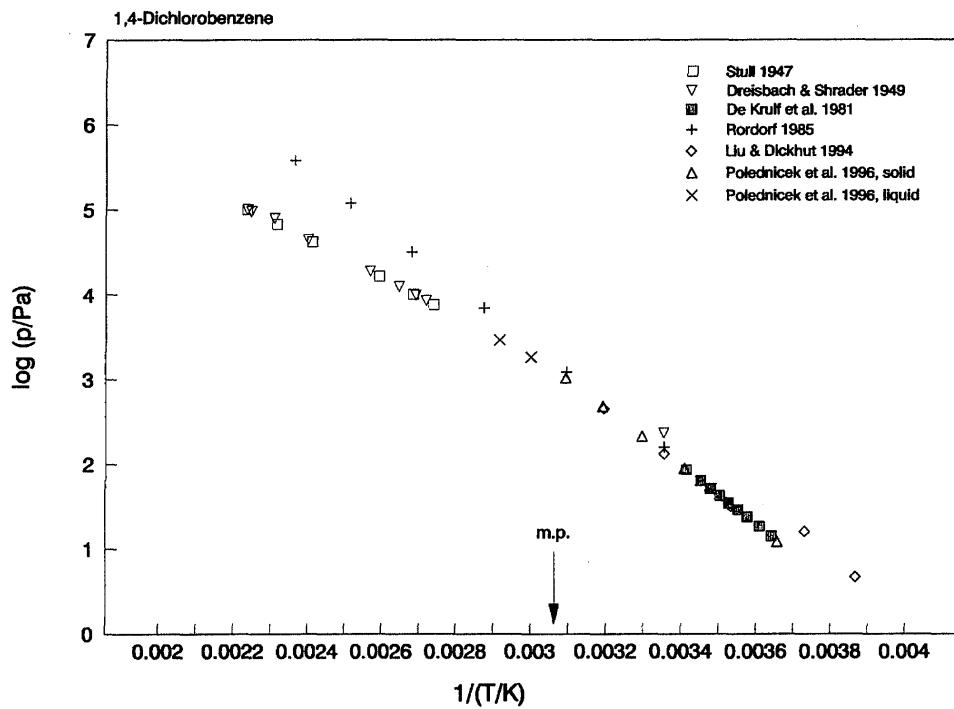
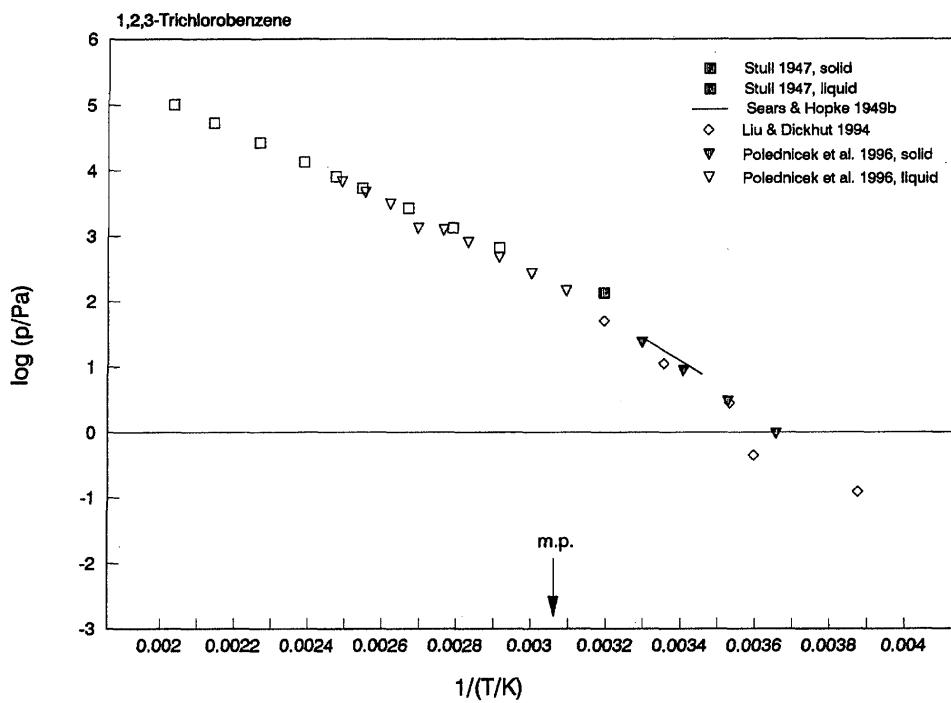
FIG. 15. Logarithm of mole fraction solubility vs $1/T$ for decachlorobiphenyl.FIG. 16. Logarithm of mole fraction solubility vs $1/T$ for dibenzo-p-dioxin.

FIG. 17. Logarithm of mole fraction solubility vs $1/T$ for 2-chlorodibenzo-*p*-dioxin.FIG. 18. Logarithm of mole fraction solubility vs $1/T$ for 1,2,3,4-tetrachlorodibenzo-*p*-dioxin.

FIG. 19. Logarithm of mole fraction solubility vs $1/T$ for 2,3,7,8-tetrachlorodibenzo-*p*-dioxin.FIG. 20. Logarithm of mole fraction solubility vs $1/T$ for octachlorodibenzo-*p*-dioxin.

FIG. 21. Logarithm of mole fraction solubility vs $1/T$ for dibenzofuran.FIG. 22. Logarithm of vapor pressure vs $1/T$ for chlorobenzene.

FIG. 23. Logarithm of vapor pressure vs $1/T$ for 1,2-dichlorobenzene.FIG. 24. Logarithm of vapor pressure vs $1/T$ for 1,3-dichlorobenzene.

FIG. 25. Logarithm of vapor pressure vs $1/T$ for 1,4-dichlorobenzene.FIG. 26. Logarithm of vapor pressure vs $1/T$ for 1,2,3-trichlorobenzene.

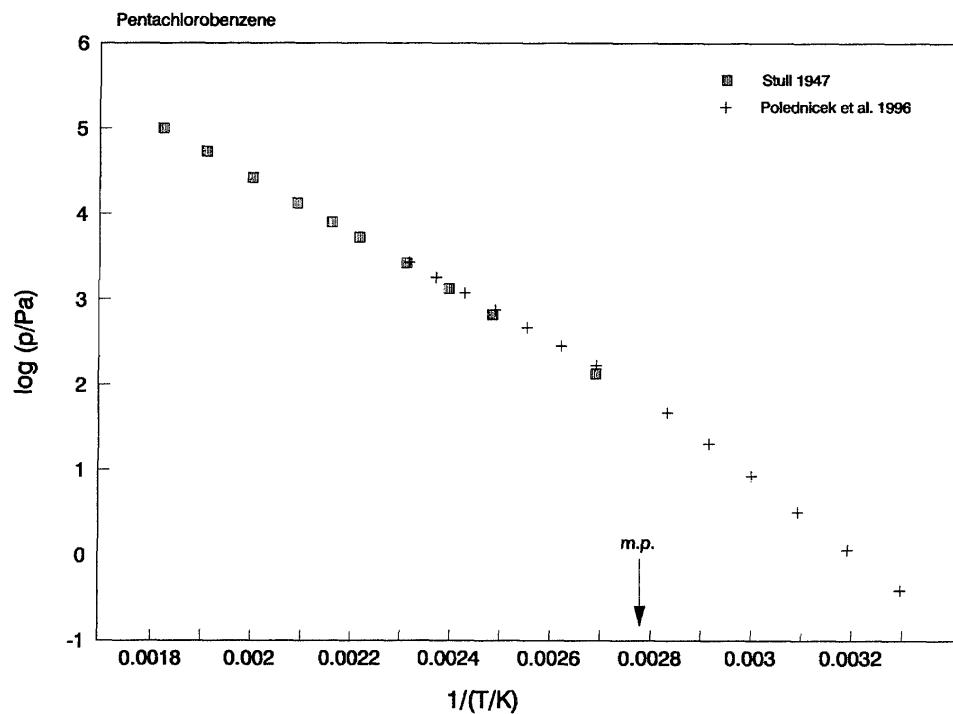
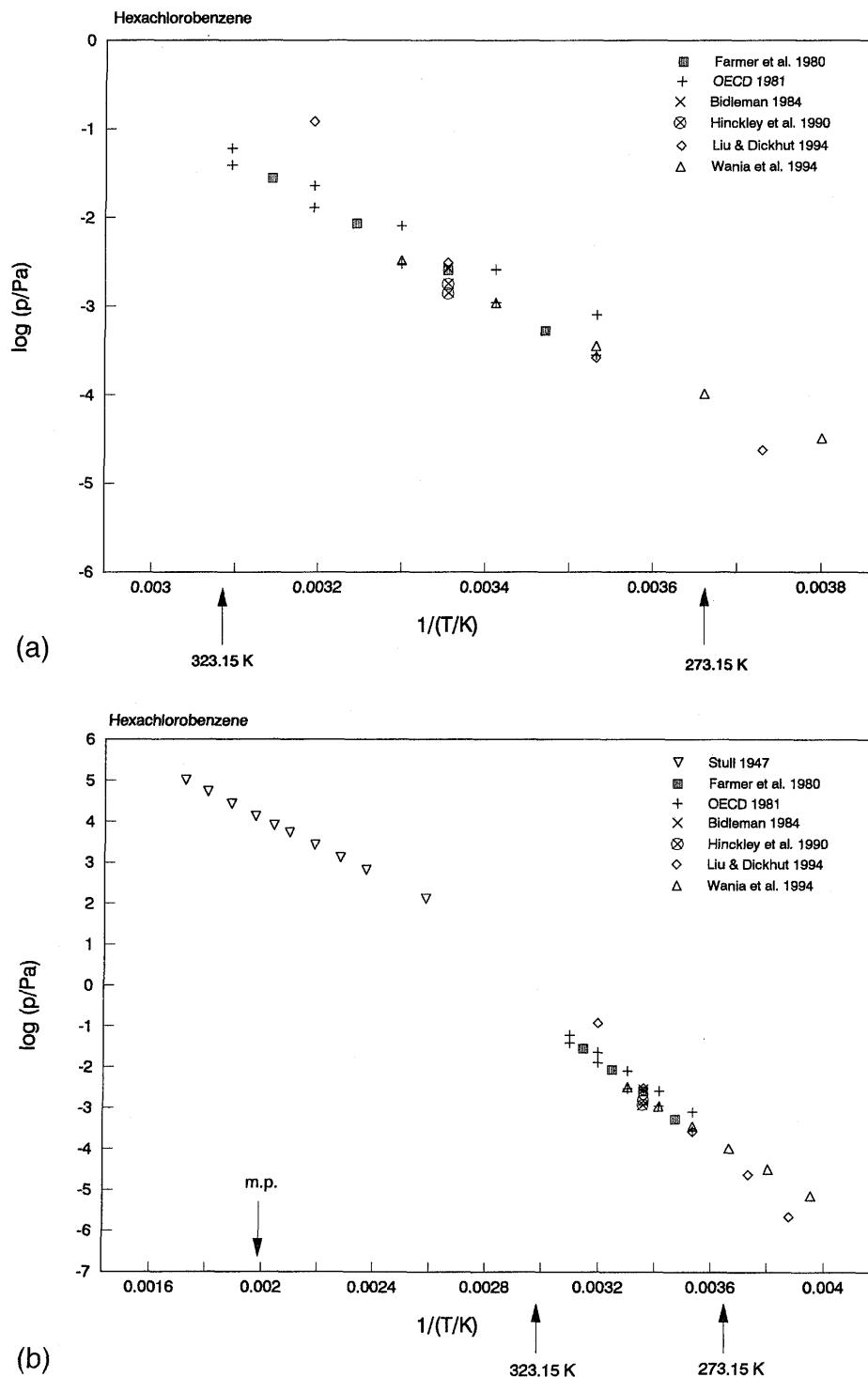


FIG. 27. Logarithm of vapor pressure vs $1/T$ for pentachlorobenzene.

FIG. 28. Logarithm of vapor pressure vs $1/T$ for hexachlorobenzene.

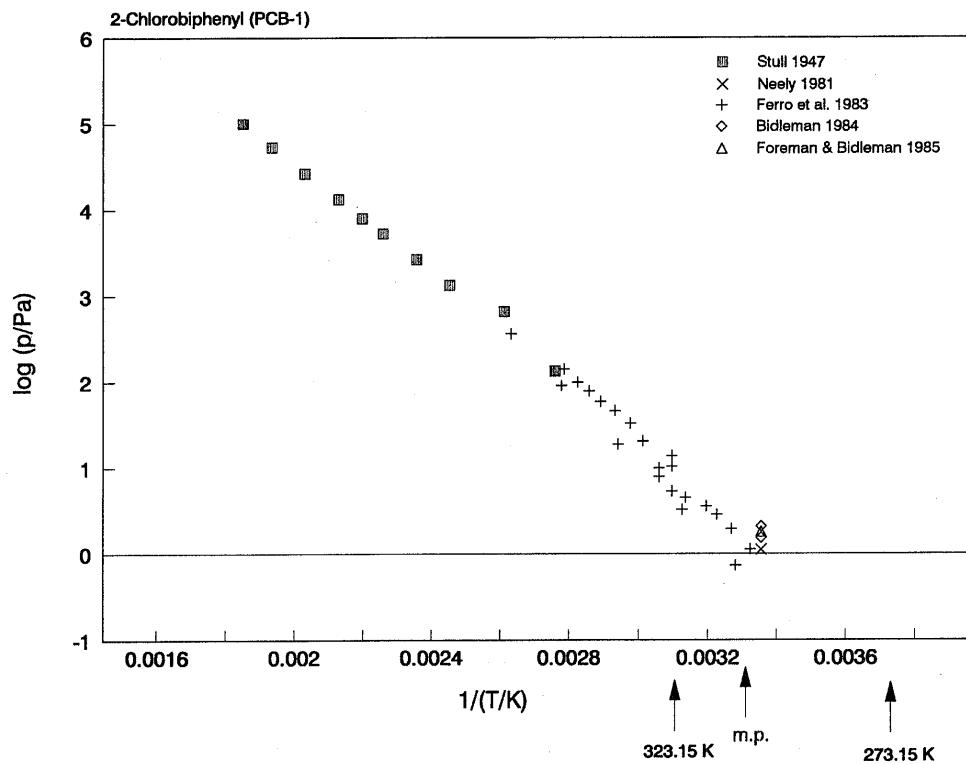
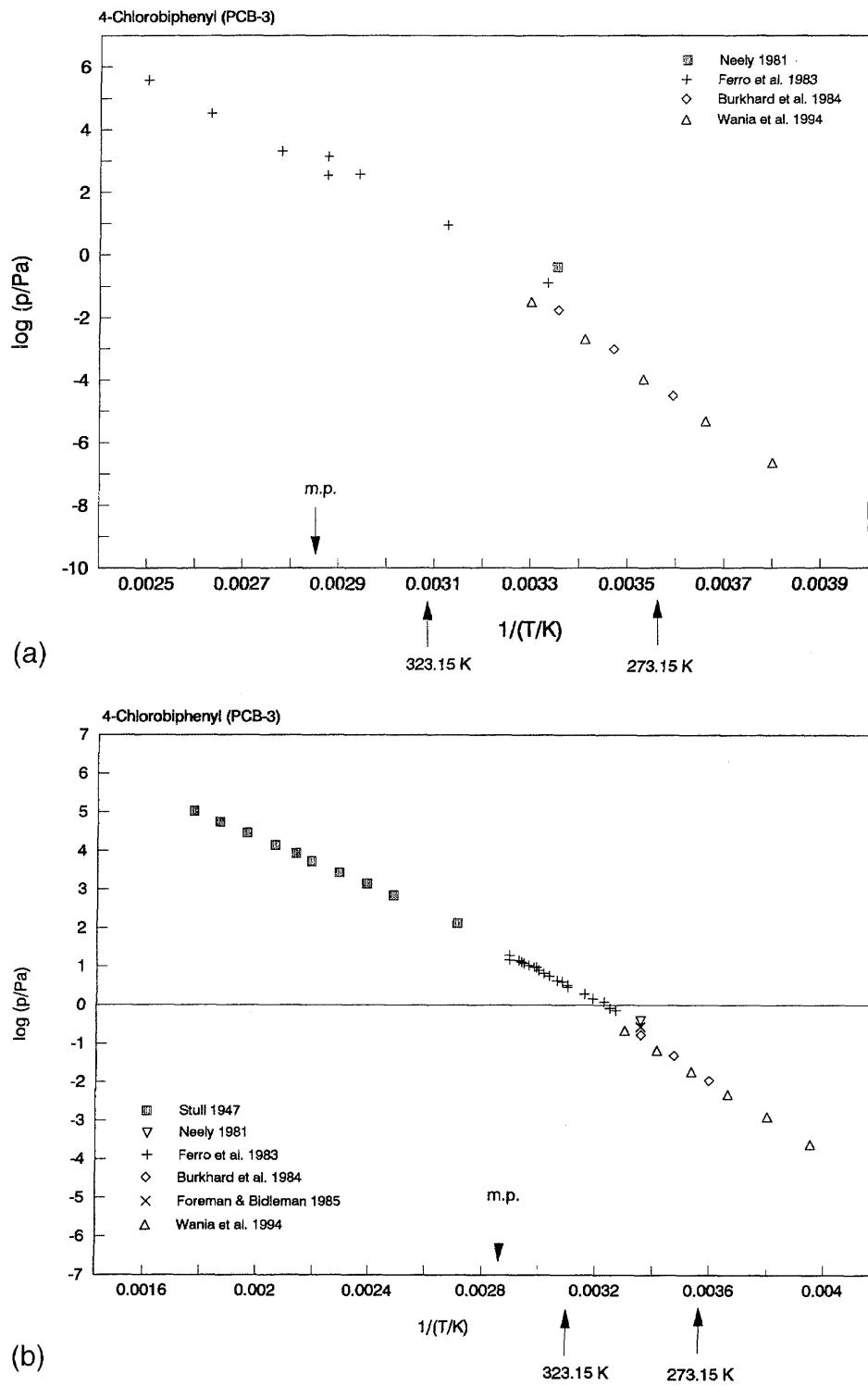


FIG. 29. Logarithm of vapor pressure vs $1/T$ for 2-chlorobiphenyl.

FIG. 30. Logarithm of vapor pressure vs $1/T$ for 4-chlorobiphenyl.

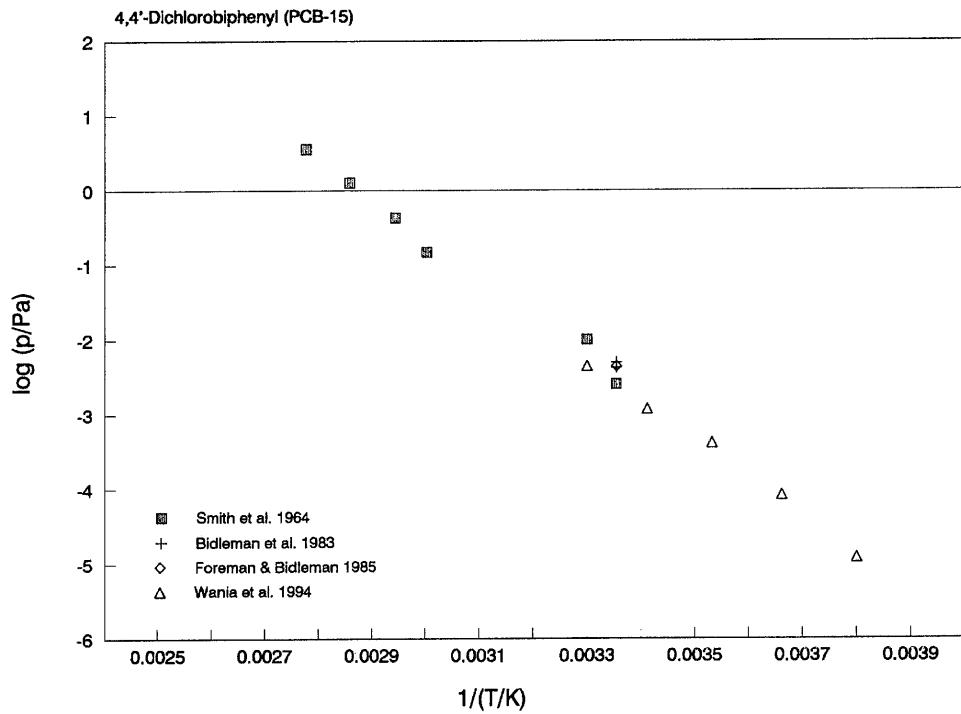


FIG. 31. Logarithm of vapor pressure vs $1/T$ for 4,4'-dichlorobiphenyl.

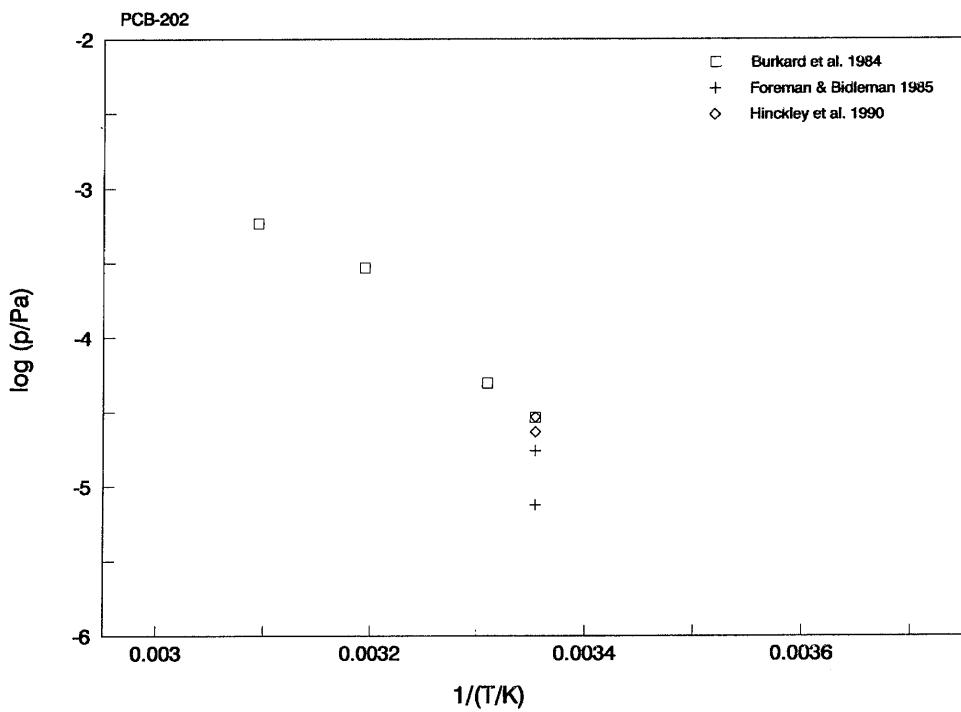


FIG. 32. Logarithm of vapor pressure vs $1/T$ for 2,2',3,3',5,5',6,6'-octachlorobiphenyl.

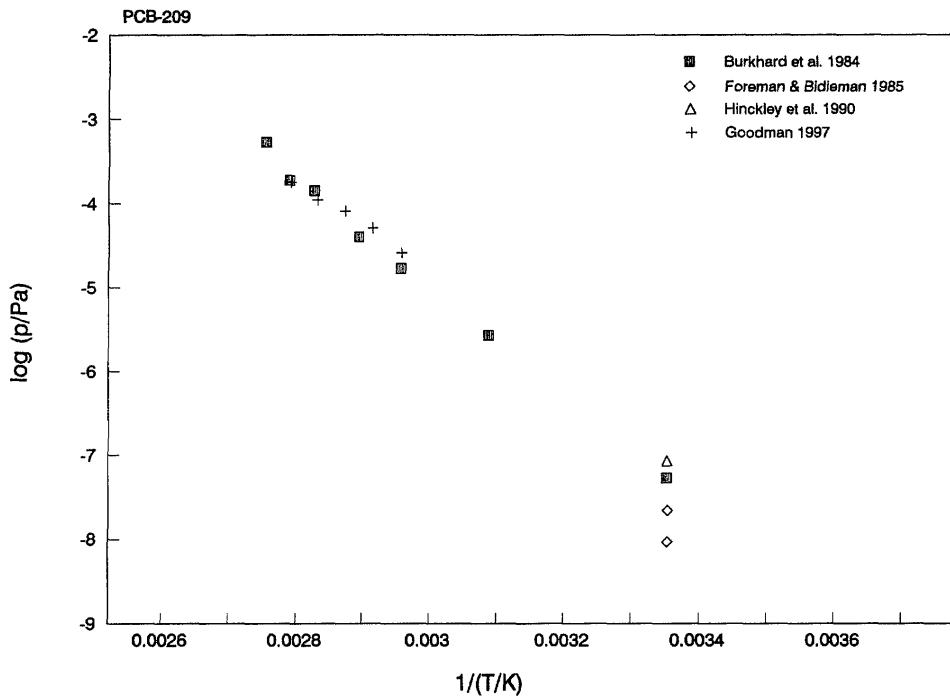
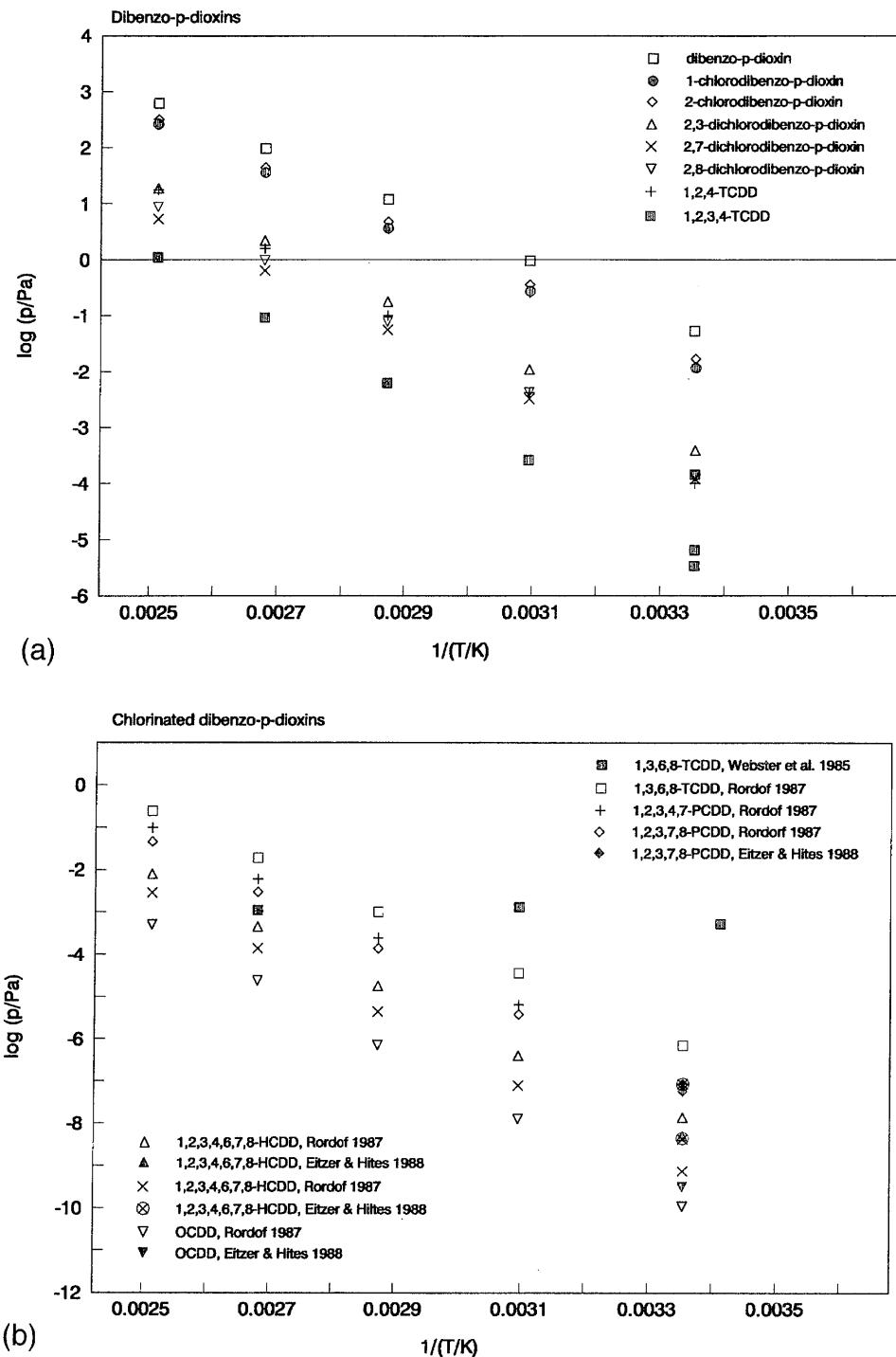
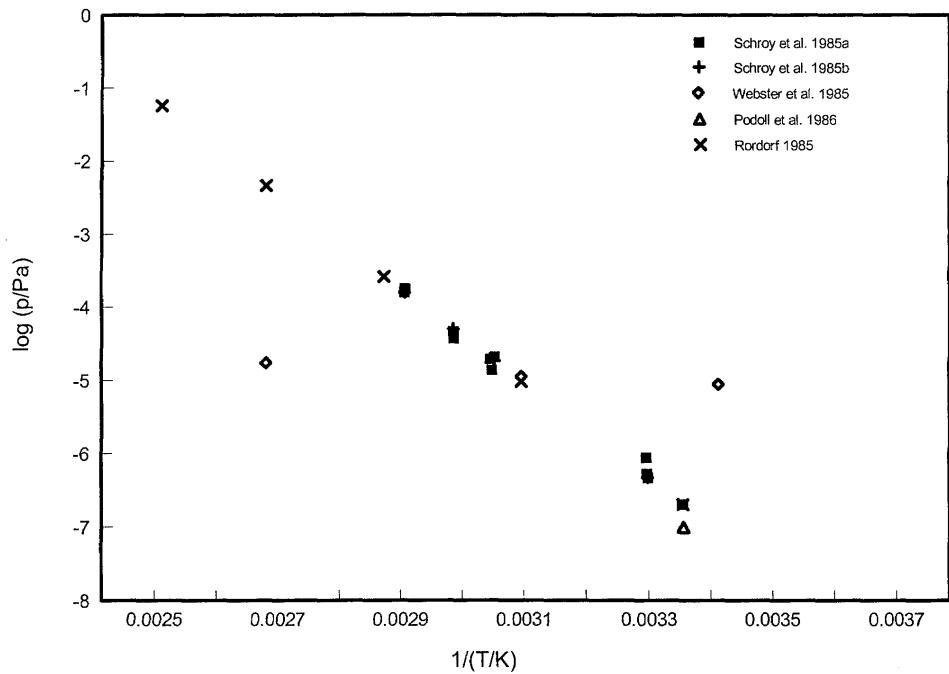
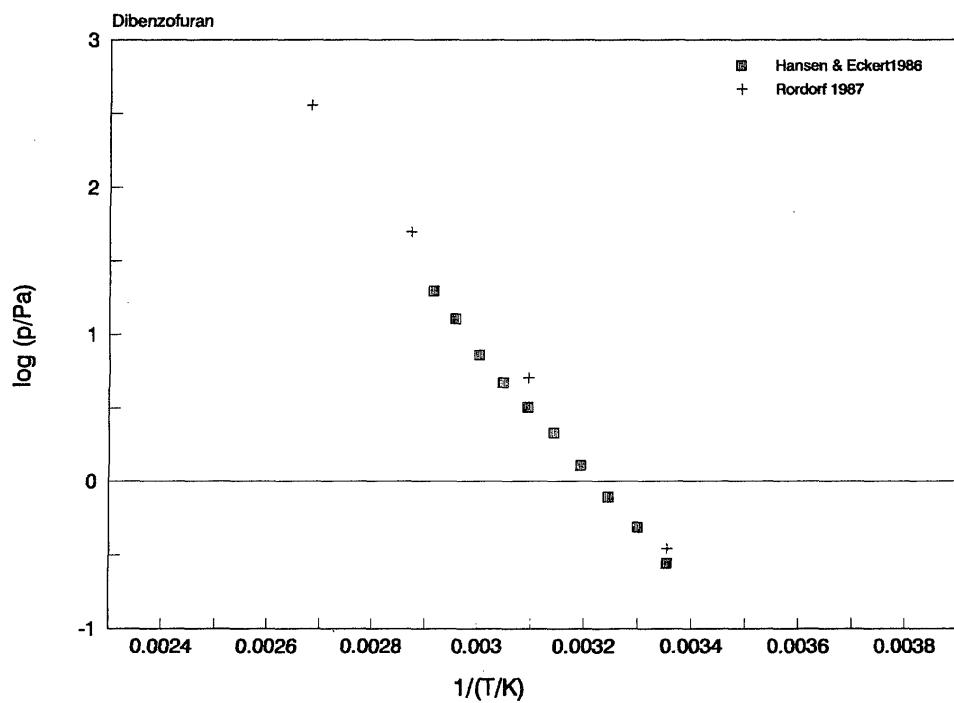
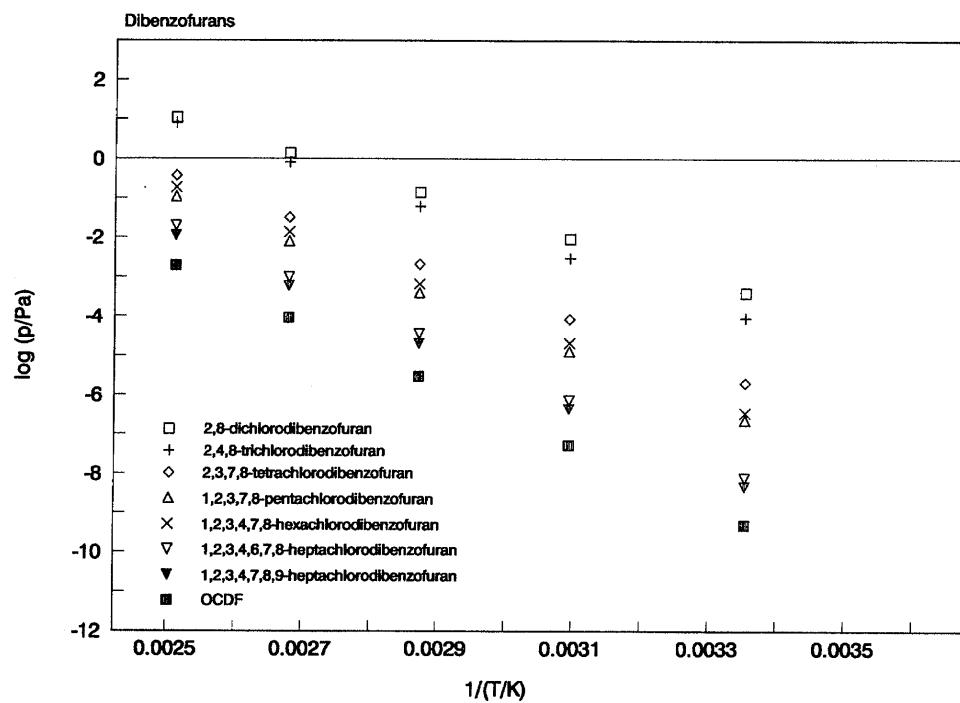
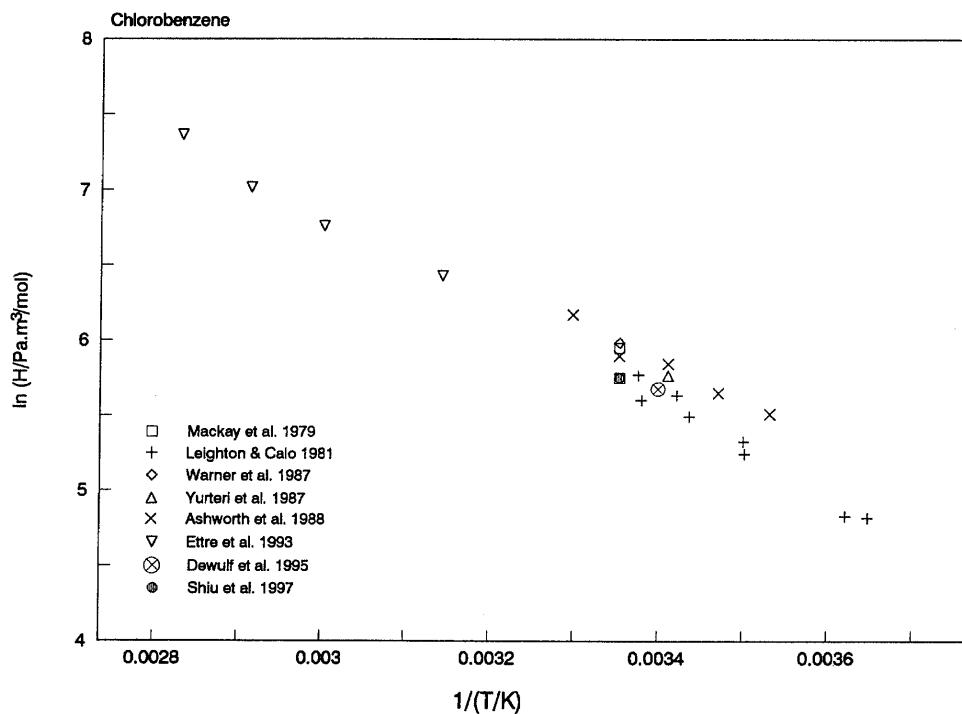
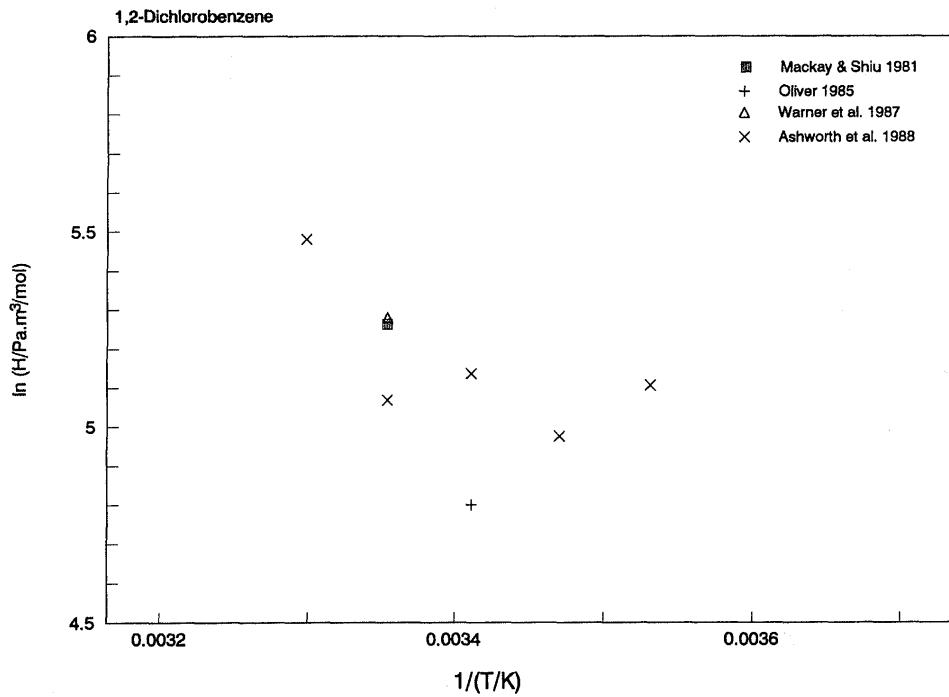
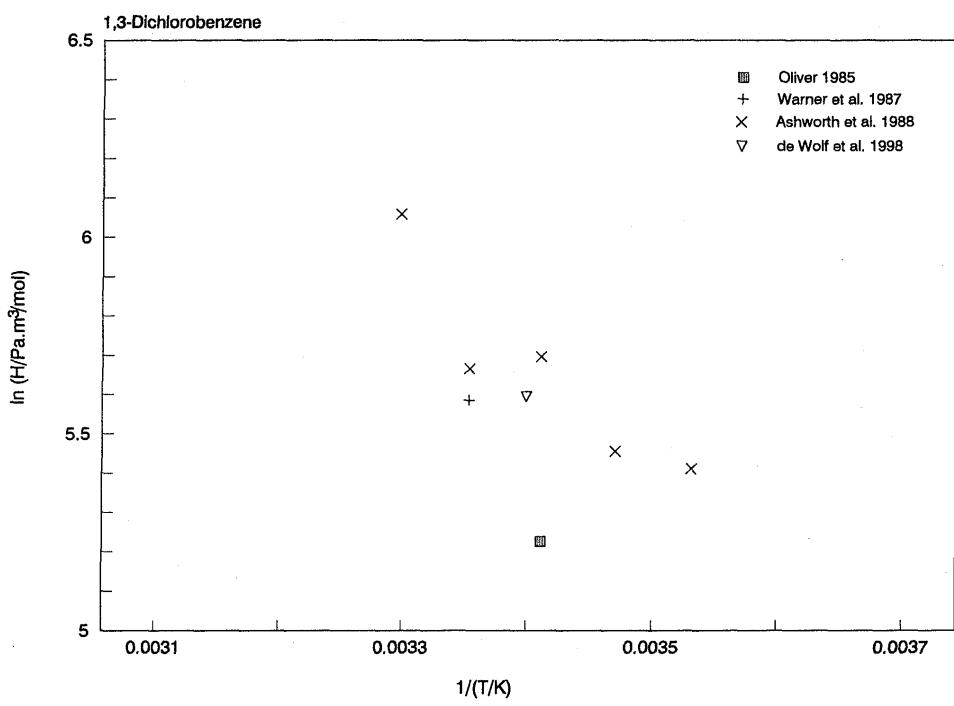


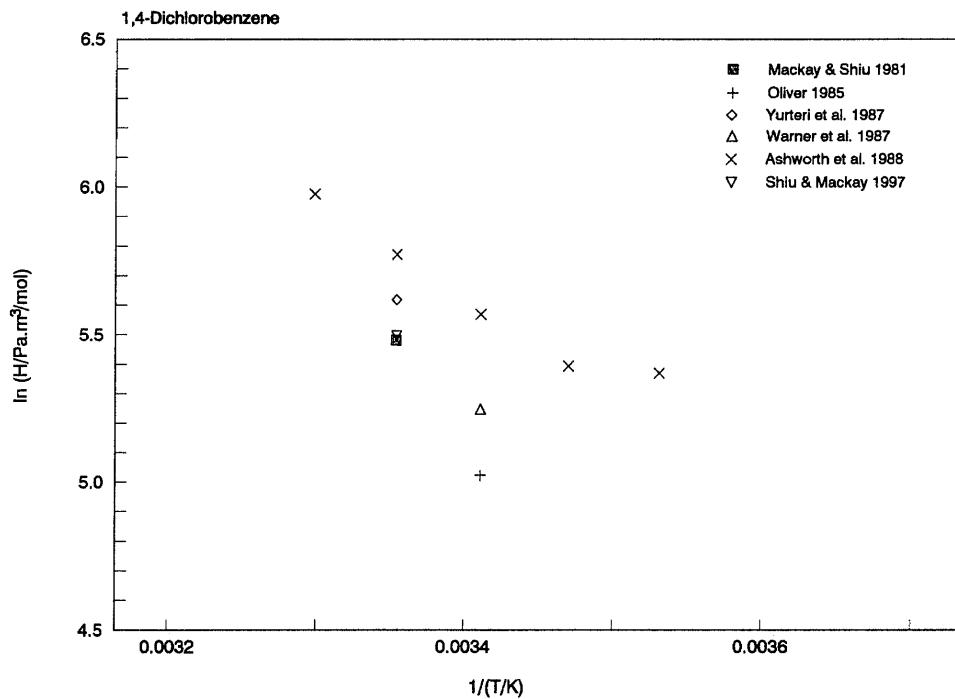
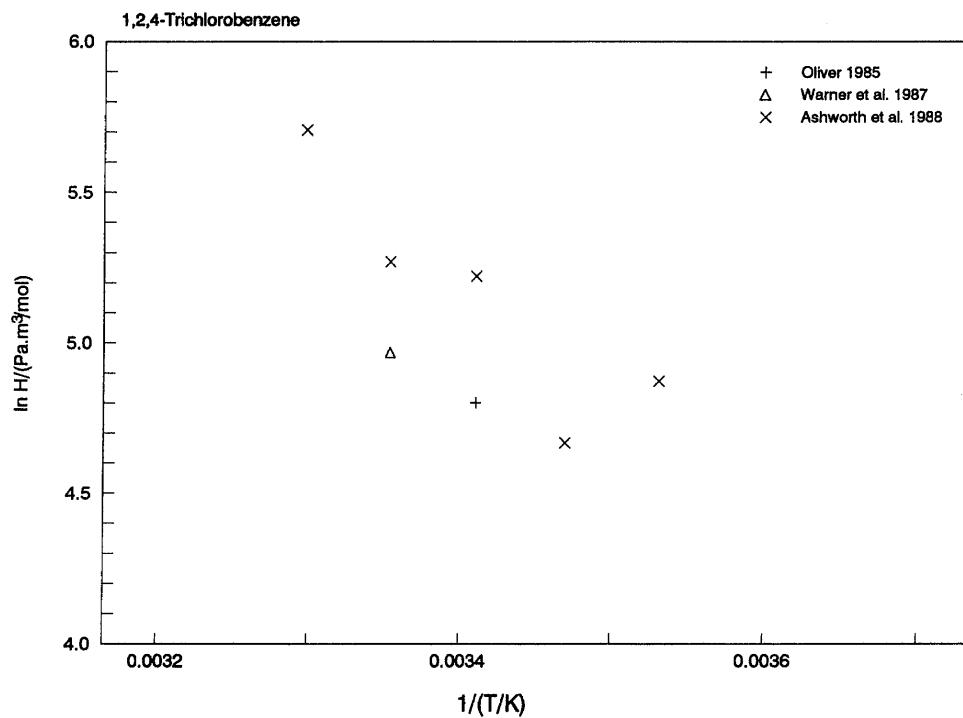
FIG. 33. Logarithm of vapor pressure vs $1/T$ for decachlorobiphenyl.

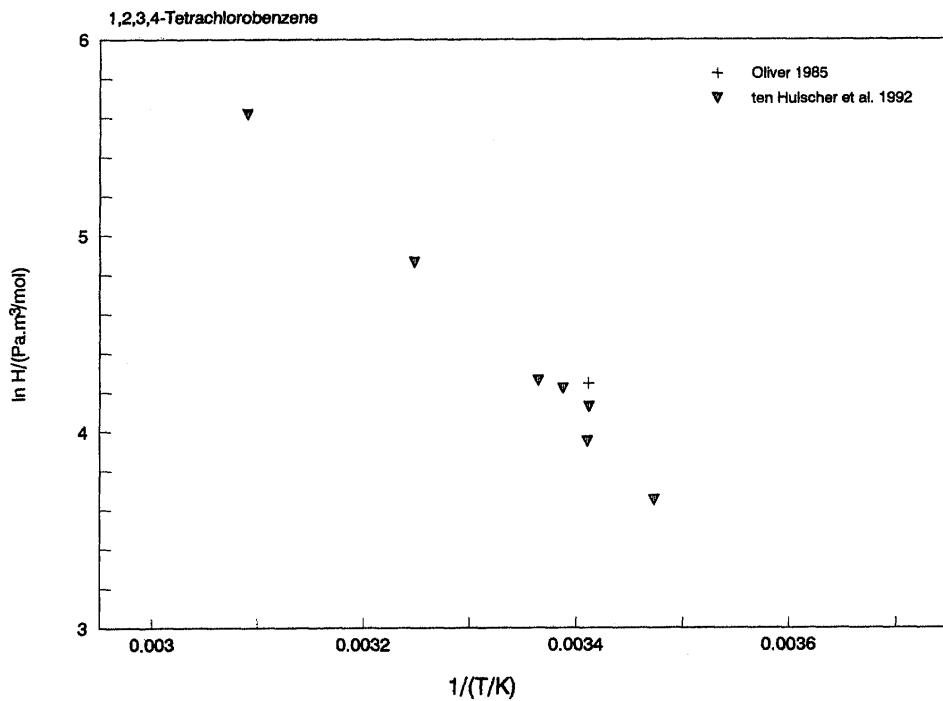
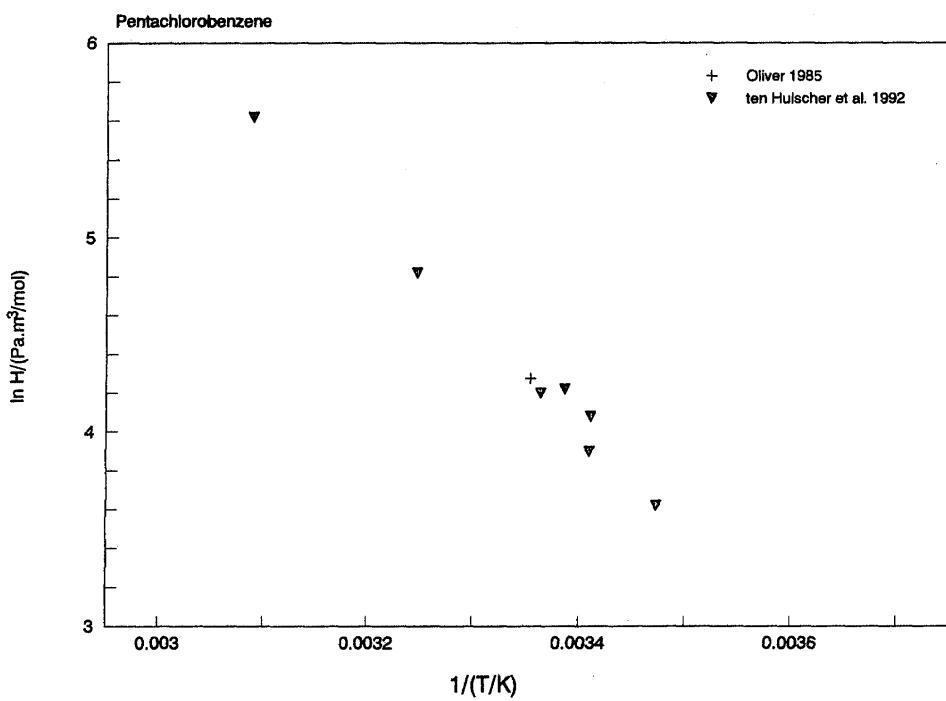
FIG. 34. Logarithm of vapor pressure vs $1/T$ for chlorinated dibenzo-*p*-dioxins.

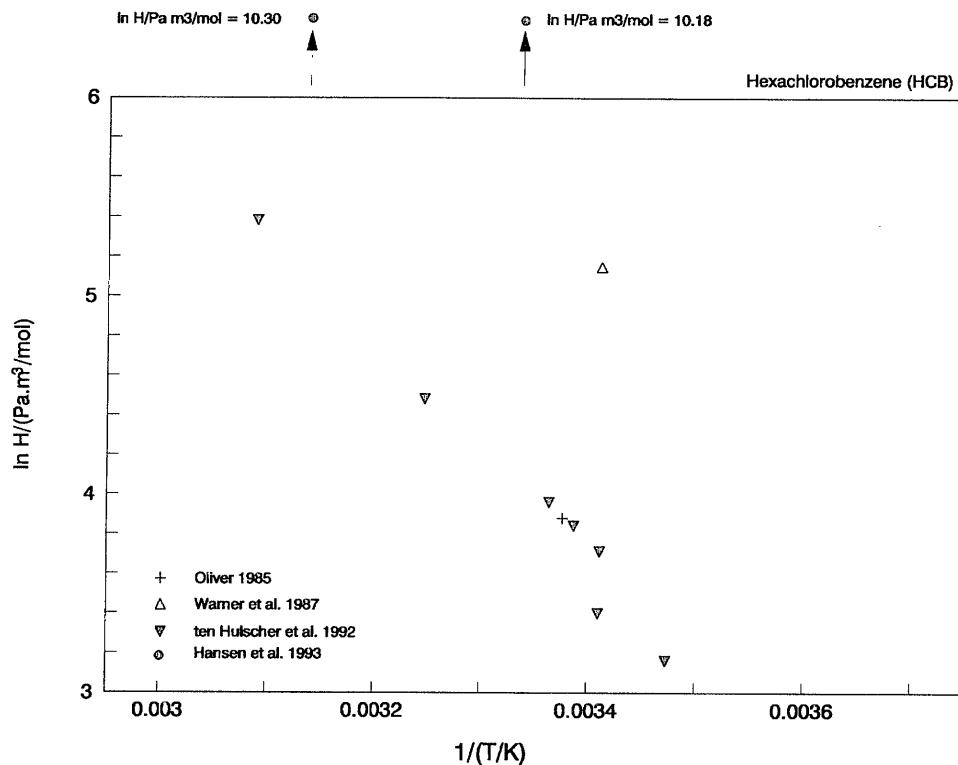
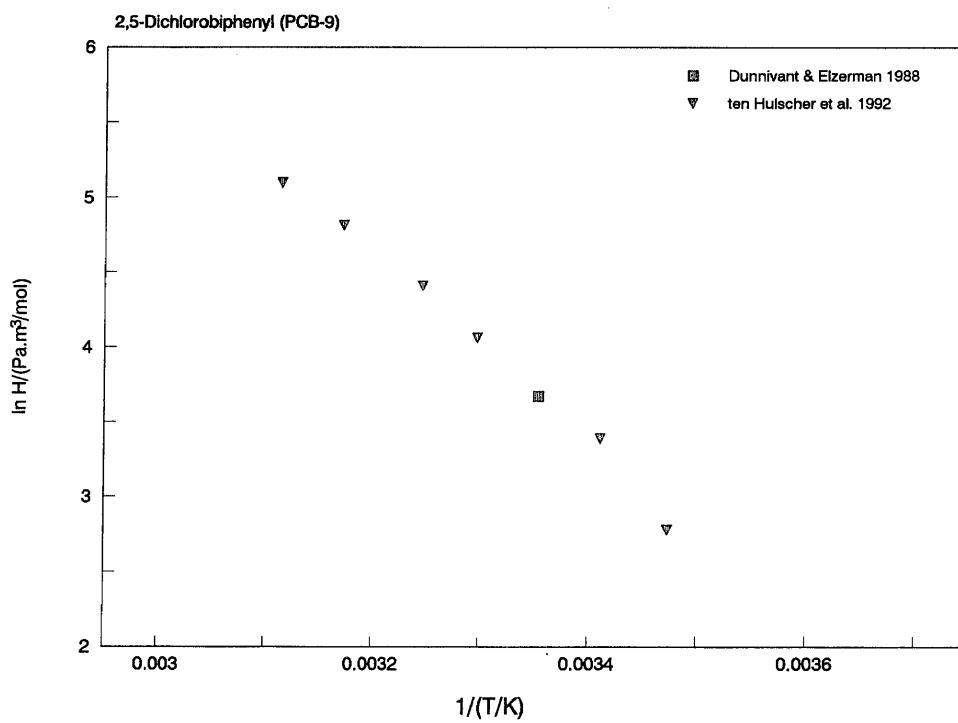
FIG. 35. Logarithm of vapor pressure vs $1/T$ for 2,3,7,8-tetrachlorodibenzo-*p*-dioxin.FIG. 36. Logarithm of vapor pressure vs $1/T$ for dibenzofuran.

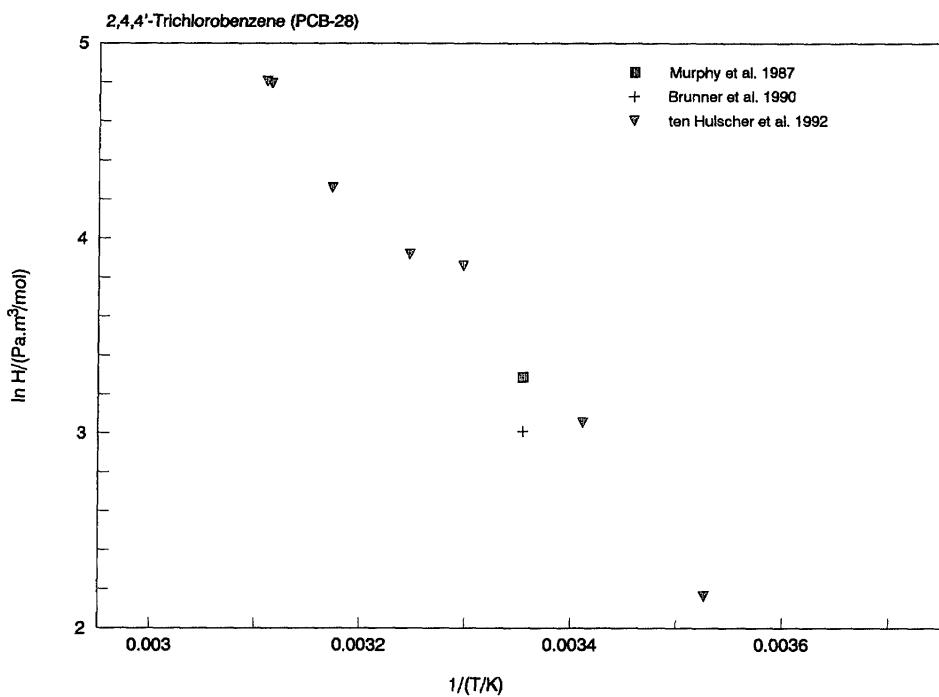
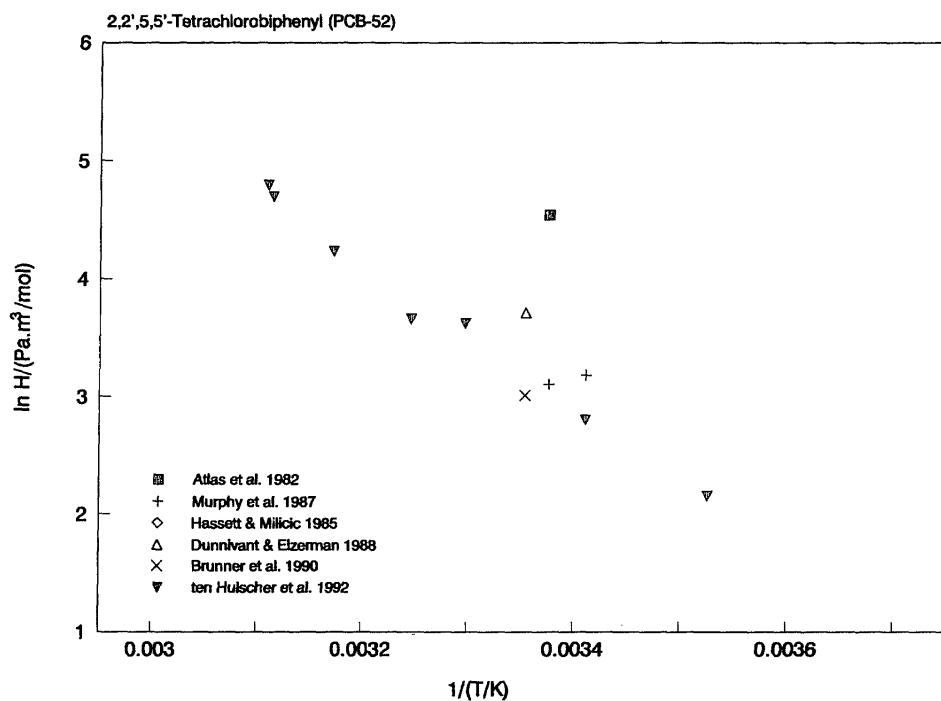
FIG. 37. Logarithm of vapor pressure vs $1/T$ for chlorinated dibenzofurans.FIG. 38. Logarithm of Henry's law constant vs $1/T$ for chlorobenzene.

FIG. 39. Logarithm of Henry's law constant vs $1/T$ for 1,2-dichlorobenzene.FIG. 40. Logarithm of Henry's law constant vs $1/T$ for 1,3-dichlorobenzene.

FIG. 41. Logarithm of Henry's law constant vs $1/T$ for 1,4-dichlorobenzene.FIG. 42. Logarithm of Henry's law constant vs $1/T$ for 1,2,4-trichlorobenzene.

FIG. 43. Logarithm of Henry's law constant vs $1/T$ for 1,2,3,4-tetrachlorobenzene.FIG. 44. Logarithm of Henry's law constant vs $1/T$ for pentachlorobenzene.

FIG. 45. Logarithm of Henry's law constant vs $1/T$ for hexachlorobenzene.FIG. 46. Logarithm of Henry's law constant vs $1/T$ for 2,5-dichlorobiphenyl.

FIG. 47. Logarithm of Henry's law constant vs $1/T$ for 2,4,4'-trichlorobiphenyl.FIG. 48. Logarithm of Henry's law constant vs $1/T$ for 2,2',5,5'-tetrachlorobiphenyl.

Whereas every effort has been made to report all quantities and equations accurately, there remains a possibility of error during data compilation. Accordingly, it is recommended that values be checked with the original reference.

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